Electronic Supplementary Material (ESI) for Dalton Transactions


# Complexation behavior of carbones containing fluorenyl ligands

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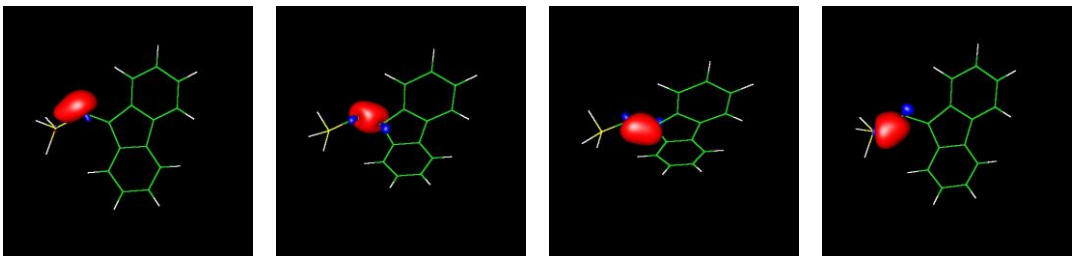
**Table S1**. Counterpoise corrections in kcal/mol for the energetically lowest lying structures **1(AuCl)** – **6(AuCl)** and **$Me_2S$(AuCl)** at the BP86/TZVPP//BP86/SVP, SCS-MP2/TZVPP//BP86/SVP and M05-2X/TZVPP//BP86/SVP levels of theory.

| | BP86/TZVPP | MP2/TZVPP | M05-2X/TZVPP |
|---|---|---|---|
| **1(AuCl)** | 0.93 | 7.47 | 1.20 |
| **2(AuCl)** | 1.12 | 9.54 | 1.43 |
| **3(AuCl)** | 0.95 | 8.02 | 1.22 |
| **4(AuCl)** | 1.03 | 8.44 | 1.36 |
| **5(AuCl)** | 0.88 | 8.99 | 1.13 |
| **6(AuCl)** | 0.98 | 9.62 | 1.23 |
| **$SMe_2$(AuCl)** | 0.70 | 4.28 | 0.91 |

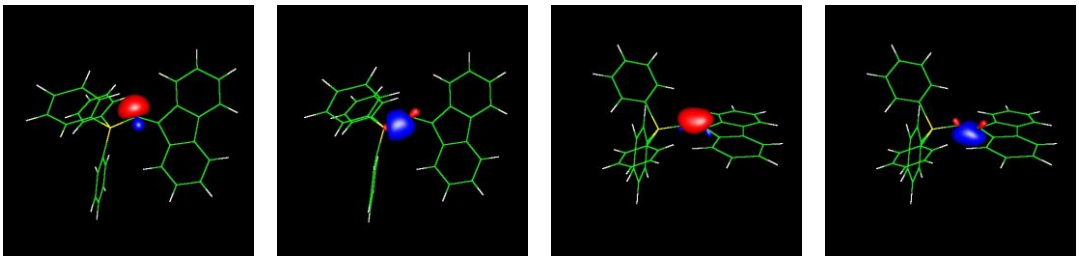
**Fig. S1**. Localised orbitals involving the central carbon atom $C_1$ in **1** – **6**

**1**:



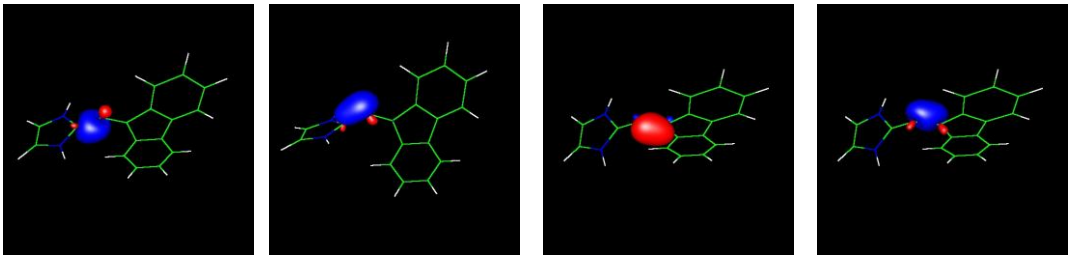
HOMO HOMO-13 HOMO-14 HOMO-24

**2**:



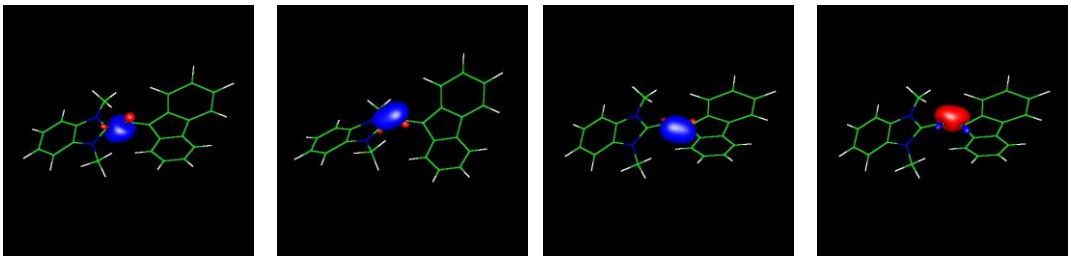
HOMO HOMO-5 HOMO-27 HOMO-31

**3**:



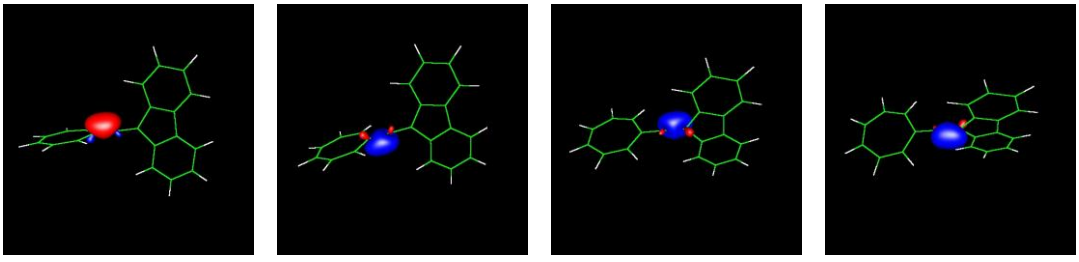
HOMO HOMO-3 HOMO-16 HOMO-17

**4**:



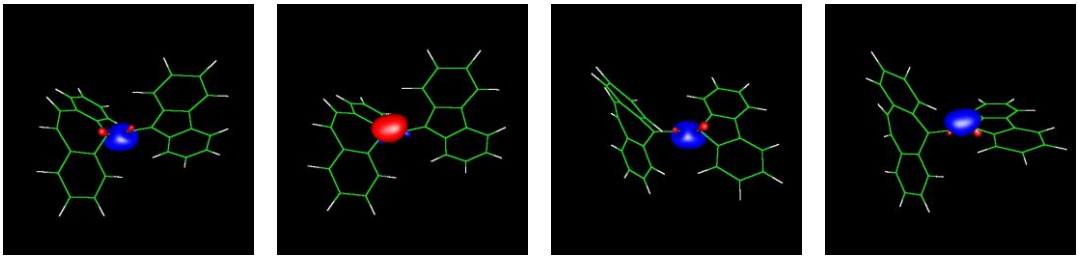
HOMO-2 HOMO-5 HOMO-20 HOMO-21

**5**:



HOMO-8 HOMO-9 HOMO-20 HOMO-21

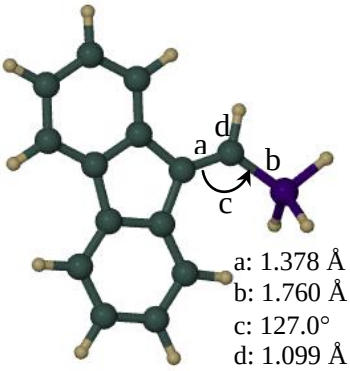
**6**:



HOMO-2 HOMO-23 HOMO-26 HOMO-27

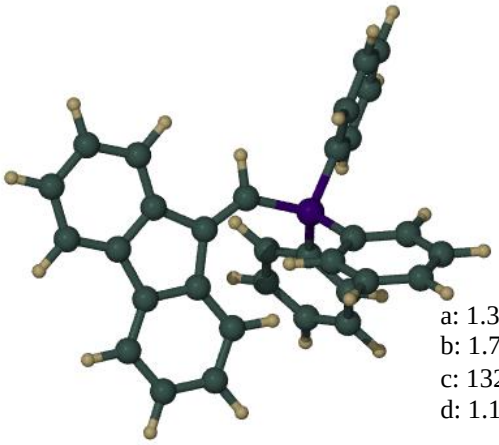
**Fig. S2**. Optimised geometries of lowest energy structures of **1(H$^+$)–6(H$^+$)** and **1(H$^+$)$_2$–6(H$^+$)$_2$** at the BP86/SVP level of theory, with important bond lengths (Å) and angles (°).

**N(H$^+$)**



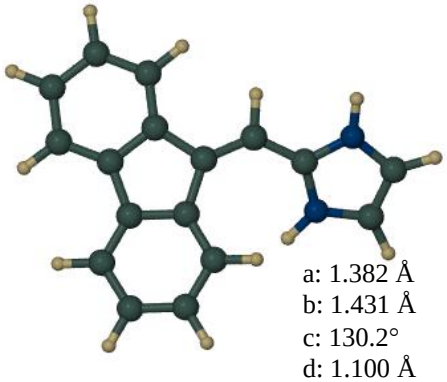

a: 1.378 Å
b: 1.760 Å
c: 127.0°
d: 1.099 Å

**1(H$^+$)**



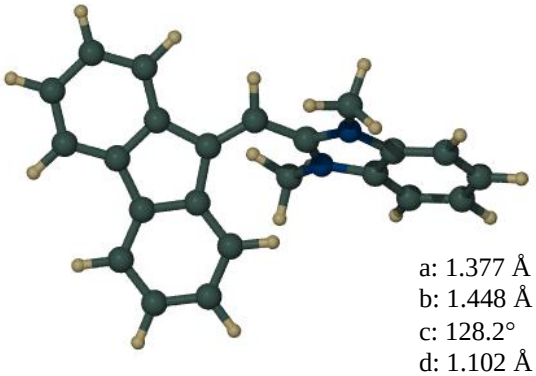
a: 1.373 Å
b: 1.794 Å
c: 132.4°
d: 1.101 Å

**2(H$^+$)**



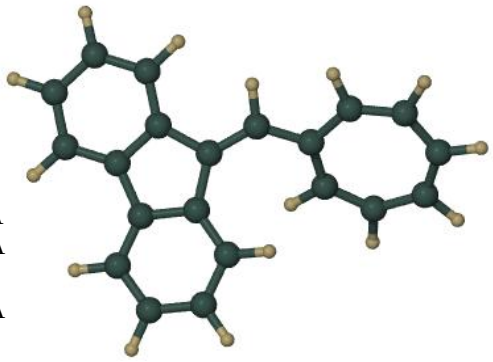
a: 1.382 Å
b: 1.431 Å
c: 130.2°
d: 1.100 Å

**3(H$^+$)**



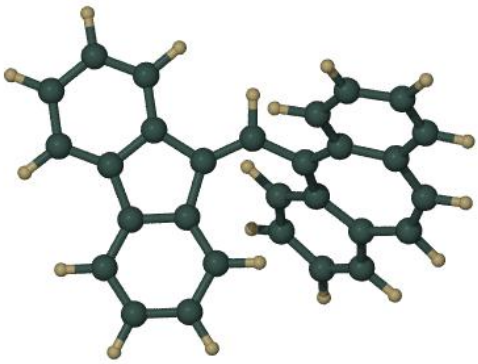
a: 1.377 Å
b: 1.448 Å
c: 128.2°
d: 1.102 Å

**4(H$^+$)**



a: 1.394 Å
b: 1.438 Å
c: 132.0°
d: 1.101 Å

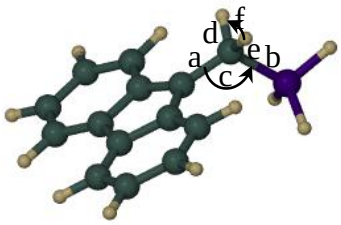
**5(H$^+$)**



a: 1.380 Å
b: 1.470 Å
c: 130.2°
d: 1.101 Å

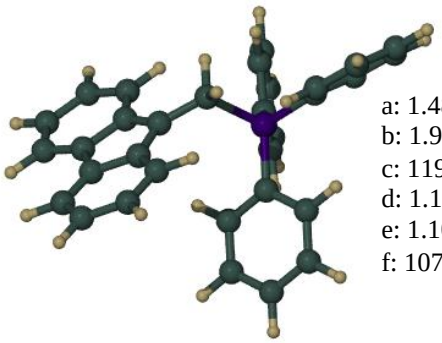
**6(H$^+$)**

**$N(H^+)_2$**




a: 1.508 Å
b: 1.845 Å
c: 115.4°
d: 1.109 Å
e: 1.109 Å
f: 107.1°

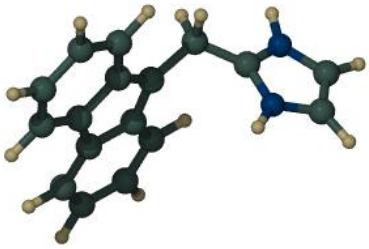
**$1(H^+)_2$**



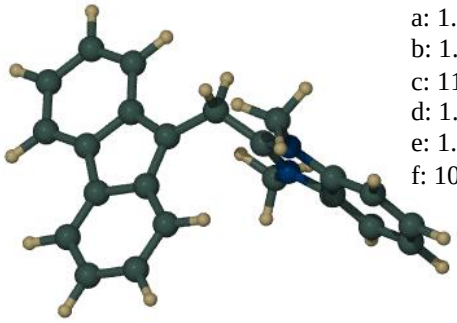
a: 1.485 Å
b: 1.902 Å
c: 119.3°
d: 1.105 Å
e: 1.107 Å
f: 107.8°

**$2(H^+)_2$**

a: 1.510 Å
b: 1.503 Å
c: 117.0°
d: 1.109 Å
e: 1.112 Å
f: 105.4°



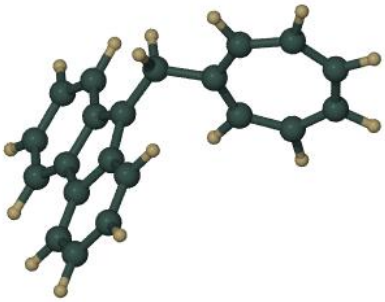
**$3(H^+)_2$**



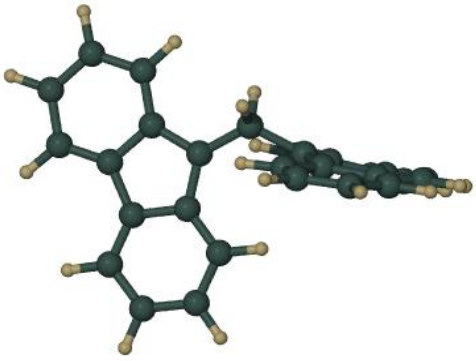
a: 1.507 Å
b: 1.503 Å
c: 118.6°
d: 1.109 Å
e: 1.111 Å
f: 104.2°

**$4(H^+)_2$**

a: 1.503 Å
b: 1.532 Å
c: 118.1°
d: 1.111 Å
e: 1.111 Å
f: 105.1°



**$5(H^+)_2$**



a: 1.500 Å
b: 1.539 Å
c: 123.0°
d: 1.108 Å
e: 1.100 Å
f: 102.2°

**$6(H^+)_2$**

**Table S2:** Geometries and SCF energies (BP86/SVP) of optimised structures of investigated molecules

**1**

Energy = -880.9450225637

| | | | |
|---|---|---|---|
| P | 9.3105099 | 15.1042120 | 4.5060990 |
| C | 9.5147649 | 18.5982613 | 3.9018355 |
| C | 8.8579717 | 17.5167414 | 3.1077060 |
| C | 8.2622298 | 18.2174245 | 1.9339366 |
| C | 7.5281060 | 17.6951005 | 0.8609845 |
| H | 7.3250415 | 16.6158724 | 0.8160797 |
| C | 7.0688190 | 18.5750074 | -0.1355928 |
| H | 6.4911040 | 18.1846663 | -0.9855665 |
| C | 7.3416075 | 19.9560924 | -0.0569423 |
| H | 6.9739929 | 20.6276324 | -0.8458656 |
| C | 8.0784273 | 20.4856266 | 1.0185177 |
| H | 8.2856068 | 21.5640909 | 1.0704525 |
| C | 8.5390309 | 19.6111508 | 2.0157406 |
| C | 9.3198517 | 19.8497190 | 3.2422216 |
| C | 9.8428476 | 21.0322195 | 3.7878490 |
| H | 9.6954191 | 21.9978038 | 3.2835103 |
| C | 10.5621272 | 20.9654553 | 4.9950223 |
| H | 10.9771092 | 21.8841898 | 5.4332028 |
| C | 10.7560619 | 19.7331697 | 5.6480065 |
| H | 11.3204902 | 19.6987978 | 6.5905295 |
| C | 10.2334498 | 18.5447851 | 5.1045067 |
| H | 10.3921761 | 17.5902530 | 5.6244961 |
| C | 8.7415930 | 16.1723307 | 3.2777040 |
| H | 10.0850433 | 15.1914038 | 5.7617118 |
| H | 8.1914254 | 14.3935417 | 5.0201222 |
| H | 10.0774275 | 14.0848160 | 3.8782097 |

**1(AuCl)**

Energy = -1477.055149762

| | | | |
|---|---|---|---|
| P | 0.7267014 | -3.1254592 | 1.4253470 |
| C | 0.5413519 | 0.2128569 | 0.9805168 |
| C | -0.1342711 | -0.8062363 | 0.1282214 |
| C | -0.6888914 | -0.0500165 | -1.0256363 |
| C | -1.4548466 | -0.4769567 | -2.1210309 |
| H | -1.7789320 | -1.5257009 | -2.1984573 |
| C | -1.8044795 | 0.4558236 | -3.1135512 |
| H | -2.4115828 | 0.1311542 | -3.9696563 |
| C | -1.3854619 | 1.7968886 | -3.0224962 |
| H | -1.6652294 | 2.5088938 | -3.8115552 |
| C | -0.6122101 | 2.2343623 | -1.9314420 |
| H | -0.2853374 | 3.2816515 | -1.8666631 |
| C | -0.2710261 | 1.3102758 | -0.9340043 |
| C | 0.4878377 | 1.4768681 | 0.3138442 |
| C | 1.0538256 | 2.6212226 | 0.8923305 |
| H | 1.0137626 | 3.5888478 | 0.3731727 |
| C | 1.6559766 | 2.5211821 | 2.1597873 |
| H | 2.1013391 | 3.4113839 | 2.6252710 |
| C | 1.6610970 | 1.2965671 | 2.8506954 |

| | | | |
|---|---|---|---|
| H | 2.0948788 | 1.2388856 | 3.8584283 |
| C | 1.0934949 | 0.1457357 | 2.2720779 |
| H | 1.0594238 | -0.7745449 | 2.8698753 |
| C | -0.2144369 | -2.1774474 | 0.2590956 |
| H | 1.8474312 | -2.5599533 | 2.1177837 |
| H | -0.0469814 | -3.6879168 | 2.4756163 |
| H | 1.3064846 | -4.2543419 | 0.7995448 |
| Cl | -2.5855119 | -5.2047904 | -1.7204285 |
| Au | -1.3043769 | -3.5892653 | -0.6868172 |

**1(AuCl)$_2$a**

Energy = -2073.121498549

| | | | |
|---|---|---|---|
| P | 0.5842504 | -2.7839943 | 1.7696325 |
| C | 0.6530709 | 0.4223300 | 0.9401792 |
| C | -0.0405558 | -0.6057698 | 0.1335878 |
| C | -0.6264191 | 0.1101217 | -1.0238925 |
| C | -1.3914506 | -0.3504212 | -2.1100391 |
| H | -1.6563560 | -1.4124744 | -2.2069448 |
| C | -1.8207958 | 0.5689071 | -3.0825812 |
| H | -2.4185321 | 0.2137297 | -3.9325934 |
| C | -1.4938103 | 1.9342248 | -2.9787562 |
| H | -1.8391398 | 2.6363361 | -3.7501229 |
| C | -0.7290080 | 2.4080196 | -1.8960773 |
| H | -0.4767079 | 3.4746742 | -1.8195636 |
| C | -0.2995284 | 1.4954642 | -0.9244459 |
| C | 0.4956921 | 1.6924412 | 0.2943968 |
| C | 1.0564175 | 2.8534336 | 0.8382138 |
| H | 0.9317574 | 3.8226997 | 0.3363045 |
| C | 1.7848201 | 2.7655991 | 2.0398049 |
| H | 2.2301821 | 3.6700212 | 2.4765022 |
| C | 1.9462969 | 1.5278624 | 2.6861259 |
| H | 2.5152601 | 1.4703640 | 3.6237707 |
| C | 1.3845482 | 0.3580961 | 2.1427415 |
| H | 1.5410924 | -0.5791375 | 2.6914478 |
| C | -0.1630108 | -1.9935643 | 0.3403934 |
| H | 0.1157731 | -2.3503085 | 3.0440650 |
| H | 0.3335405 | -4.1720660 | 1.7607032 |
| H | 2.0020757 | -2.6819605 | 1.8739383 |
| Cl | -4.2085921 | -3.6253441 | 0.5983279 |
| Au | -2.0560772 | -2.9428270 | 0.2021823 |
| Cl | 1.3687350 | -4.5789740 | -2.8311286 |
| Au | 0.2763914 | -3.3475433 | -1.2361523 |

**1(AuCl)$_2$b**

Energy = -2073.118671611

| | | | |
|---|---|---|---|
| C | -1.7830719 | 1.4517079 | -3.3827869 |
| C | -1.1055623 | 1.9307174 | -2.2517379 |
| C | -1.3012737 | 3.2694400 | -1.8093202 |
| C | -2.1833545 | 4.1225398 | -2.4865077 |
| C | -2.8618120 | 3.6339831 | -3.6181753 |
| C | -2.6610032 | 2.3140314 | -4.0630616 |
| C | -0.1565914 | 1.2472624 | -1.3183179 |

| | | | |
|---|---|---|---|
| C | 0.2747458 | 2.3095505 | -0.3479926 |
| C | -0.4526130 | 3.5033179 | -0.6317063 |
| C | -0.2637130 | 4.6574535 | 0.1416001 |
| C | 0.6728790 | 4.6312211 | 1.1902553 |
| C | 1.4267500 | 3.4721103 | 1.4460336 |
| C | 1.2388078 | 2.3111506 | 0.6738856 |
| C | -0.0627353 | -0.1806767 | -1.2203460 |
| P | 0.4996980 | -1.0643022 | 0.2317218 |
| Au | -1.1375140 | -1.6417333 | -2.1518816 |
| Cl | -2.3659813 | -3.2977498 | -3.1699440 |
| Au | 1.6394758 | 0.3913425 | -2.3995632 |
| Cl | 3.5620812 | 0.3205569 | -3.6215602 |
| H | -1.6300023 | 0.4215023 | -3.7354686 |
| H | -3.1931116 | 1.9500453 | -4.9521594 |
| H | -3.5551627 | 4.2908119 | -4.1615775 |
| H | -2.3454863 | 5.1538279 | -2.1439158 |
| H | -0.8283882 | 5.5747304 | -0.0743833 |
| H | 0.8340512 | 5.5307306 | 1.8002509 |
| H | 2.1833102 | 3.4757899 | 2.2422499 |
| H | 1.8880851 | 1.4451405 | 0.8531560 |
| H | -0.5917482 | -1.4372116 | 1.0583201 |
| H | 1.4218637 | -0.5079991 | 1.1765072 |
| H | 1.1164576 | -2.2739964 | -0.1543561 |

**1(AuCl)$_2$c**

Energy = -2073.095823638

| | | | |
|---|---|---|---|
| C | 1.1178330 | 2.4055566 | 0.7855256 |
| C | 0.2502420 | 2.4668795 | -0.3137436 |
| C | -0.4689499 | 3.6612320 | -0.6083568 |
| C | -0.3216592 | 4.7912748 | 0.2084616 |
| C | 0.5458823 | 4.7221823 | 1.3148698 |
| C | 1.2601321 | 3.5439401 | 1.6009127 |
| C | -1.2871389 | 3.4326065 | -1.8128319 |
| C | -1.0759994 | 2.0963588 | -2.2555609 |
| C | -0.1035802 | 1.4300779 | -1.3331003 |
| C | -2.1820833 | 4.2658665 | -2.4987553 |
| C | -2.8539579 | 3.7548167 | -3.6255240 |
| C | -2.6401122 | 2.4332976 | -4.0603238 |
| C | -1.7435510 | 1.5908630 | -3.3785066 |
| C | 0.1063560 | 0.0293238 | -1.2885143 |
| Au | -0.8990607 | -1.8075748 | -1.8963378 |
| Cl | -1.9557657 | -3.7381800 | -2.5351678 |
| Au | 1.7213544 | 0.7703054 | -2.4289636 |
| Cl | 3.6471623 | 0.9064804 | -3.6386759 |
| P | 0.5044599 | -1.1700146 | -0.0055504 |
| H | -1.5773569 | 0.5558660 | -3.7086605 |
| H | -3.1748207 | 2.0573578 | -4.9431086 |
| H | -3.5597277 | 4.3957956 | -4.1719267 |
| H | -2.3665167 | 5.2960850 | -2.1643188 |
| H | -0.8753626 | 5.7163590 | -0.0036588 |
| H | 0.6733744 | 5.6031067 | 1.9592916 |
| H | 1.9386167 | 3.5134960 | 2.4643902 |

| | | | |
|---|---|---|---|
| H | 1.6989906 | 1.4975475 | 0.9969835 |
| H | -0.5550389 | -1.6387221 | 0.8127416 |
| H | 1.3835775 | -0.7760187 | 1.0888229 |
| H | 1.3216039 | -2.2317591 | -0.4546520 |

**1($H^+$)**

Energy = -881.3752734306

| | | | |
|---|---|---|---|
| P | 0.4485898 | -3.1135124 | 1.7022519 |
| C | 0.6465720 | 0.1984147 | 0.9575176 |
| C | -0.0633280 | -0.8208400 | 0.1546442 |
| C | -0.6505175 | -0.1119999 | -1.0014491 |
| C | -1.4201716 | -0.5949504 | -2.0705593 |
| H | -1.6852837 | -1.6580266 | -2.1567991 |
| C | -1.8573800 | 0.3148799 | -3.0510417 |
| H | -2.4604498 | -0.0421199 | -3.8958474 |
| C | -1.5267991 | 1.6789059 | -2.9561136 |
| H | -1.8769468 | 2.3741493 | -3.7308957 |
| C | -0.7525839 | 2.1706298 | -1.8824682 |
| H | -0.5042164 | 3.2386048 | -1.8247074 |
| C | -0.3166359 | 1.2702607 | -0.9073300 |
| C | 0.4922993 | 1.4651708 | 0.3138501 |
| C | 1.0666400 | 2.6149565 | 0.8612497 |
| H | 0.9529079 | 3.5918418 | 0.3732586 |
| C | 1.8019813 | 2.5031498 | 2.0607107 |
| H | 2.2585972 | 3.3996594 | 2.5011743 |
| C | 1.9598868 | 1.2621794 | 2.7010191 |
| H | 2.5358848 | 1.1965561 | 3.6329193 |
| C | 1.3818649 | 0.1023551 | 2.1511938 |
| H | 1.5293664 | -0.8487840 | 2.6829187 |
| C | -0.2035555 | -2.1755929 | 0.3633692 |
| H | -0.0064256 | -2.7536940 | 3.0001625 |
| H | 0.0684301 | -4.4656557 | 1.5369377 |
| H | 1.8650540 | -3.1363074 | 1.8219766 |
| H | -0.7749315 | -2.7871021 | -0.3490033 |

**1($H^+$)$_2$**

Energy = -881.5899071836

| | | | |
|---|---|---|---|
| P | -0.6278878 | -2.8127890 | 1.4436049 |
| C | 1.0403123 | 0.4706168 | 0.7997613 |
| C | 0.3588577 | -0.5452006 | 0.0479181 |
| C | -0.4960656 | 0.0727258 | -0.9262738 |
| C | -1.3316752 | -0.4895741 | -1.9269977 |
| H | -1.4141309 | -1.5764936 | -2.0713426 |
| C | -2.0520071 | 0.3751489 | -2.7672992 |
| H | -2.7015752 | -0.0326596 | -3.5521207 |
| C | -1.9310531 | 1.7686508 | -2.6127857 |
| H | -2.4961714 | 2.4341551 | -3.2804345 |
| C | -1.0835466 | 2.3492815 | -1.6159833 |
| H | -1.0112421 | 3.4420186 | -1.5362614 |
| C | -0.3717107 | 1.5029969 | -0.7832909 |
| C | 0.6018935 | 1.7551415 | 0.3104665 |
| C | 1.1163336 | 2.9190018 | 0.8554825 |

| | | | |
|---|---|---|---|
| H | 0.8066393 | 3.9128624 | 0.5061679 |
| C | 2.0872700 | 2.8093222 | 1.9015924 |
| H | 2.5034465 | 3.7289980 | 2.3363206 |
| C | 2.5291020 | 1.5615905 | 2.3794012 |
| H | 3.2850251 | 1.5177878 | 3.1736481 |
| C | 2.0125850 | 0.3765590 | 1.8302126 |
| H | 2.3818001 | -0.5933509 | 2.1935767 |
| C | 0.5300088 | -2.0312515 | 0.2381427 |
| H | -1.9803255 | -2.6510860 | 1.0569553 |
| H | -0.3585586 | -4.2019785 | 1.5237163 |
| H | -0.4875867 | -2.2644725 | 2.7414585 |
| H | 0.3801196 | -2.5840368 | -0.7113842 |
| H | 1.5462122 | -2.2815368 | 0.6046079 |

**2**

Energy = -1573.653441652

| | | | |
|---|---|---|---|
| P | 0.0072660 | -1.0717907 | 0.3009409 |
| C | 0.2293353 | 2.6007445 | -0.2866955 |
| C | -0.3511382 | 1.4594602 | -1.0616471 |
| C | -0.9183767 | 2.0951233 | -2.2909538 |
| C | -1.5839147 | 1.5051301 | -3.3737262 |
| H | -1.7456561 | 0.4175677 | -3.3839496 |
| C | -2.0302200 | 2.3257701 | -4.4256552 |
| H | -2.5542986 | 1.8798656 | -5.2832559 |
| C | -1.8120375 | 3.7181542 | -4.3918375 |
| H | -2.1679685 | 4.3438985 | -5.2228727 |
| C | -1.1442688 | 4.3164004 | -3.3072084 |
| H | -0.9790546 | 5.4033324 | -3.2899300 |
| C | -0.6973976 | 3.5000943 | -2.2556470 |
| C | 0.0175735 | 3.8157120 | -1.0074699 |
| C | 0.4697659 | 5.0406891 | -0.4932810 |
| H | 0.3078114 | 5.9769469 | -1.0466160 |
| C | 1.1362113 | 5.0545196 | 0.7454575 |
| H | 1.4959166 | 6.0069375 | 1.1605514 |
| C | 1.3465245 | 3.8587173 | 1.4581403 |
| H | 1.8689610 | 3.8852781 | 2.4249350 |
| C | 0.8952562 | 2.6274205 | 0.9470463 |
| H | 1.0640504 | 1.7017058 | 1.5095177 |
| C | -0.4303805 | 0.1224066 | -0.8467657 |
| C | -2.7665612 | -1.5391606 | 0.1605835 |
| C | -1.5644628 | -1.9042281 | 0.7987280 |
| C | -1.5740836 | -2.9243402 | 1.7738087 |
| C | -2.7766070 | -3.5679629 | 2.1070855 |
| C | -3.9756266 | -3.1926629 | 1.4780326 |
| C | -3.9684026 | -2.1750943 | 0.5090784 |
| H | -2.7324029 | -0.7590661 | -0.6135986 |
| H | -0.6463537 | -3.2135039 | 2.2866281 |
| H | -2.7759349 | -4.3641027 | 2.8648446 |
| H | -4.9164846 | -3.6959606 | 1.7423194 |
| H | -4.9039732 | -1.8776235 | 0.0148427 |
| H | 0.3177231 | 0.1910449 | 5.1489990 |
| C | 0.8856479 | -0.0843318 | 4.2489692 |

| | | | |
|---|---|---|---|
| H | 2.8259922 | 0.2457156 | 5.1775716 |
| C | 2.2908136 | -0.0526649 | 4.2651938 |
| H | 4.1068936 | -0.3716201 | 3.1102699 |
| C | 3.0079725 | -0.3994489 | 3.1071051 |
| H | 2.8987828 | -1.0390279 | 1.0388159 |
| C | 2.3265311 | -0.7813602 | 1.9411328 |
| C | 0.9132197 | -0.8312700 | 1.9197665 |
| C | 0.2001665 | -0.4655889 | 3.0851368 |
| H | -0.8988736 | -0.4748629 | 3.0819642 |
| H | 2.1661462 | -2.9418011 | -3.7846730 |
| C | 2.0126281 | -3.0746120 | -2.7044719 |
| H | 3.1742633 | -4.9112046 | -2.6031020 |
| C | 2.5787301 | -4.1769798 | -2.0421807 |
| H | 2.8193164 | -5.2018909 | -0.1379352 |
| C | 2.3798138 | -4.3408546 | -0.6609272 |
| H | 1.4904554 | -3.5311193 | 1.1417697 |
| C | 1.6225240 | -3.4026846 | 0.0585802 |
| C | 1.0505766 | -2.2967177 | -0.6055668 |
| C | 1.2412604 | -2.1423222 | -1.9931018 |
| H | 0.7663292 | -1.2867559 | -2.4947467 |

**2(AuCl)**

Energy = -2169.757661876

| | | | |
|---|---|---|---|
| P | -0.1185146 | -1.0970762 | 0.2366824 |
| C | -0.2109601 | 2.4492176 | -0.1079221 |
| C | -0.5467007 | 1.4066202 | -1.1224839 |
| C | -0.6693373 | 2.1543906 | -2.4109912 |
| C | -0.9926323 | 1.7182480 | -3.7060070 |
| H | -1.2825942 | 0.6708811 | -3.8815521 |
| C | -0.9568059 | 2.6353968 | -4.7711804 |
| H | -1.2233974 | 2.2974904 | -5.7823138 |
| C | -0.5885443 | 3.9773643 | -4.5568468 |
| H | -0.5641483 | 4.6790484 | -5.4026598 |
| C | -0.2532147 | 4.4257227 | -3.2670114 |
| H | 0.0382849 | 5.4726319 | -3.1009374 |
| C | -0.2995735 | 3.5157493 | -2.2006761 |
| C | -0.0386125 | 3.7055437 | -0.7693752 |
| C | 0.2475133 | 4.8723527 | -0.0462612 |
| H | 0.3800084 | 5.8327547 | -0.5642305 |
| C | 0.3293489 | 4.8051162 | 1.3558000 |
| H | 0.5477955 | 5.7128563 | 1.9359390 |
| C | 0.0933566 | 3.5884708 | 2.0210101 |
| H | 0.1162318 | 3.5520091 | 3.1190812 |
| C | -0.1889384 | 2.4157504 | 1.2969494 |
| H | -0.4068238 | 1.4940676 | 1.8462983 |
| C | -0.7098783 | 0.0363839 | -1.0206860 |
| C | -2.5748635 | -1.0715153 | 1.5383596 |
| C | -1.5660414 | -1.9101450 | 1.0135518 |
| C | -1.7108730 | -3.3102252 | 1.0770508 |
| C | -2.8532294 | -3.8650941 | 1.6759677 |
| C | -3.8489070 | -3.0318966 | 2.2100687 |
| C | -3.7095133 | -1.6352153 | 2.1387975 |

| | | | |
|---|---|---|---|
| H | -2.4868637 | 0.0211589 | 1.4534631 |
| H | -0.9510511 | -3.9681396 | 0.6360905 |
| H | -2.9700060 | -4.9569126 | 1.7104812 |
| H | -4.7443708 | -3.4714511 | 2.6709673 |
| H | -4.4954120 | -0.9795044 | 2.5379853 |
| H | 1.2756720 | -0.4643575 | 5.0294832 |
| C | 1.5313919 | -0.2973709 | 3.9737991 |
| H | 3.4192306 | 0.6825187 | 4.4194976 |
| C | 2.7328440 | 0.3427888 | 3.6313160 |
| H | 4.0007329 | 1.0448916 | 2.0076424 |
| C | 3.0606791 | 0.5450924 | 2.2789472 |
| H | 2.4540576 | 0.2693910 | 0.2155453 |
| C | 2.1898943 | 0.1109294 | 1.2706312 |
| C | 0.9750875 | -0.5233947 | 1.6122832 |
| C | 0.6499287 | -0.7314100 | 2.9685459 |
| H | -0.2897875 | -1.2300463 | 3.2421748 |
| H | 2.3733381 | -3.3367397 | -3.5107345 |
| C | 2.1550055 | -3.3344077 | -2.4341467 |
| H | 3.4308815 | -5.0408671 | -2.0041231 |
| C | 2.7472774 | -4.2864318 | -1.5901510 |
| H | 2.9392766 | -5.0039338 | 0.4562029 |
| C | 2.4707092 | -4.2686083 | -0.2125103 |
| H | 1.4212130 | -3.2774354 | 1.4013310 |
| C | 1.6032643 | -3.3022989 | 0.3178684 |
| C | 0.9820281 | -2.3610011 | -0.5353497 |
| C | 1.2705484 | -2.3749554 | -1.9145936 |
| H | 0.7932909 | -1.6438800 | -2.5809960 |
| Cl | -3.1749633 | -2.4933188 | -3.5599896 |
| Au | -1.8023326 | -1.1671745 | -2.2460727 |

**2$(AuCl)_2$a**

| | | | |
|---|---|---|---|
| P | 0.3083172 | -1.1141321 | 0.1705408 |
| C | 0.2761677 | 2.4283160 | -0.3358360 |
| C | -0.1009876 | 1.3715972 | -1.3408248 |
| C | -1.0760184 | 2.0591051 | -2.2605885 |
| C | -1.6985065 | 1.6288035 | -3.4423280 |
| H | -1.4539441 | 0.6496859 | -3.8800752 |
| C | -2.6349912 | 2.4698308 | -4.0701020 |
| H | -3.1160889 | 2.1373624 | -5.0000497 |
| C | -2.9541042 | 3.7271191 | -3.5253795 |
| H | -3.6921048 | 4.3683691 | -4.0275810 |
| C | -2.3273160 | 4.1739492 | -2.3488335 |
| H | -2.5710606 | 5.1597020 | -1.9284368 |
| C | -1.3827781 | 3.3440540 | -1.7275229 |
| C | -0.5399438 | 3.5779838 | -0.5486114 |
| C | -0.3915381 | 4.7230855 | 0.2471088 |
| H | -1.0260070 | 5.6052313 | 0.0829167 |
| C | 0.6103948 | 4.7418838 | 1.2333686 |
| H | 0.7462110 | 5.6368435 | 1.8567904 |
| C | 1.4698540 | 3.6407567 | 1.3945786 |
| H | 2.2850840 | 3.6857210 | 2.1294448 |
| C | 1.3153884 | 2.4855106 | 0.6059169 |

| | | | |
|---|---|---|---|
| H | 2.0341283 | 1.6645431 | 0.7020684 |
| C | 0.0374733 | -0.0621450 | -1.2959106 |
| C | -2.5283266 | -0.9794094 | 0.3143356 |
| C | -1.3412256 | -1.4553172 | 0.9083716 |
| C | -1.4091929 | -2.2008768 | 2.1087653 |
| C | -2.6536577 | -2.4789031 | 2.6933275 |
| C | -3.8344055 | -2.0034173 | 2.0979177 |
| C | -3.7681813 | -1.2506589 | 0.9152797 |
| H | -2.4866136 | -0.4118188 | -0.6243825 |
| H | -0.4915502 | -2.5599825 | 2.5945765 |
| H | -2.6987085 | -3.0661965 | 3.6208588 |
| H | -4.8082100 | -2.2200456 | 2.5589031 |
| H | -4.6869630 | -0.8747280 | 0.4453213 |
| H | 0.9676843 | 1.1582435 | 4.5757267 |
| C | 1.4538757 | 0.5878292 | 3.7723633 |
| H | 3.4156306 | 0.6245912 | 4.7108823 |
| C | 2.8253057 | 0.2913431 | 3.8459083 |
| H | 4.5102041 | -0.6755524 | 2.8655881 |
| C | 3.4392139 | -0.4362538 | 2.8133571 |
| H | 3.1765065 | -1.4570315 | 0.9224228 |
| C | 2.6864748 | -0.8733448 | 1.7117710 |
| C | 1.3084842 | -0.5753863 | 1.6319183 |
| C | 0.6975324 | 0.1637314 | 2.6703722 |
| H | -0.3701801 | 0.4131928 | 2.6198735 |
| H | 3.7844387 | -3.8152969 | -2.1635750 |
| C | 2.8626776 | -3.8537219 | -1.5675021 |
| H | 2.7359465 | -6.0239012 | -1.5874335 |
| C | 2.2728728 | -5.0874600 | -1.2470331 |
| H | 0.6023351 | -6.0798793 | -0.2711328 |
| C | 1.0808411 | -5.1196273 | -0.5072407 |
| H | -0.4717556 | -3.9677841 | 0.4673625 |
| C | 0.4774911 | -3.9264848 | -0.0807892 |
| C | 1.0703761 | -2.6857453 | -0.3967812 |
| C | 2.2689877 | -2.6555998 | -1.1464580 |
| H | 2.7256720 | -1.6988001 | -1.4399556 |
| Cl | 3.7920461 | 0.7283026 | -3.4283126 |
| Au | 1.7762165 | 0.6574971 | -2.3438670 |
| Cl | -1.7129304 | -2.8922135 | -4.1277927 |
| Au | -0.7863216 | -1.4023003 | -2.6236117 |

**2$(AuCl)_2$b**

Energy = -2765.821832325

| | | | |
|---|---|---|---|
| P | 0.3083172 | -1.1141321 | 0.1705408 |
| C | 0.2761677 | 2.4283160 | -0.3358360 |
| C | -0.1009876 | 1.3715972 | -1.3408248 |
| C | -1.0760184 | 2.0591051 | -2.2605885 |
| C | -1.6985065 | 1.6288035 | -3.4423280 |
| H | -1.4539441 | 0.6496859 | -3.8800752 |
| C | -2.6349912 | 2.4698308 | -4.0701020 |
| H | -3.1160889 | 2.1373624 | -5.0000497 |
| C | -2.9541042 | 3.7271191 | -3.5253795 |
| H | -3.6921048 | 4.3683691 | -4.0275810 |

| | | | |
|---|---|---|---|
| C | -2.3273160 | 4.1739492 | -2.3488335 |
| H | -2.5710606 | 5.1597020 | -1.9284368 |
| C | -1.3827781 | 3.3440540 | -1.7275229 |
| C | -0.5399438 | 3.5779838 | -0.5486114 |
| C | -0.3915381 | 4.7230855 | 0.2471088 |
| H | -1.0260070 | 5.6052313 | 0.0829167 |
| C | 0.6103948 | 4.7418838 | 1.2333686 |
| H | 0.7462110 | 5.6368435 | 1.8567904 |
| C | 1.4698540 | 3.6407567 | 1.3945786 |
| H | 2.2850840 | 3.6857210 | 2.1294448 |
| C | 1.3153884 | 2.4855106 | 0.6059169 |
| H | 2.0341283 | 1.6645431 | 0.7020684 |
| C | 0.0374733 | -0.0621450 | -1.2959106 |
| C | -2.5283266 | -0.9794094 | 0.3143356 |
| C | -1.3412256 | -1.4553172 | 0.9083716 |
| C | -1.4091929 | -2.2008768 | 2.1087653 |
| C | -2.6536577 | -2.4789031 | 2.6933275 |
| C | -3.8344055 | -2.0034173 | 2.0979177 |
| C | -3.7681813 | -1.2506589 | 0.9152797 |
| H | -2.4866136 | -0.4118188 | -0.6243825 |
| H | -0.4915502 | -2.5599825 | 2.5945765 |
| H | -2.6987085 | -3.0661965 | 3.6208588 |
| H | -4.8082100 | -2.2200456 | 2.5589031 |
| H | -4.6869630 | -0.8747280 | 0.4453213 |
| H | 0.9676843 | 1.1582435 | 4.5757267 |
| C | 1.4538757 | 0.5878292 | 3.7723633 |
| H | 3.4156306 | 0.6245912 | 4.7108823 |
| C | 2.8253057 | 0.2913431 | 3.8459083 |
| H | 4.5102041 | -0.6755524 | 2.8655881 |
| C | 3.4392139 | -0.4362538 | 2.8133571 |
| H | 3.1765065 | -1.4570315 | 0.9224228 |
| C | 2.6864748 | -0.8733448 | 1.7117710 |
| C | 1.3084842 | -0.5753863 | 1.6319183 |
| C | 0.6975324 | 0.1637314 | 2.6703722 |
| H | -0.3701801 | 0.4131928 | 2.6198735 |
| H | 3.7844387 | -3.8152969 | -2.1635750 |
| C | 2.8626776 | -3.8537219 | -1.5675021 |
| H | 2.7359465 | -6.0239012 | -1.5874335 |
| C | 2.2728728 | -5.0874600 | -1.2470331 |
| H | 0.6023351 | -6.0798793 | -0.2711328 |
| C | 1.0808411 | -5.1196273 | -0.5072407 |
| H | -0.4717556 | -3.9677841 | 0.4673625 |
| C | 0.4774911 | -3.9264848 | -0.0807892 |
| C | 1.0703761 | -2.6857453 | -0.3967812 |
| C | 2.2689877 | -2.6555998 | -1.1464580 |
| H | 2.7256720 | -1.6988001 | -1.4399556 |
| Cl | 3.7920461 | 0.7283026 | -3.4283126 |
| Au | 1.7762165 | 0.6574971 | -2.3438670 |
| Cl | -1.7129304 | -2.8922135 | -4.1277927 |
| Au | -0.7863216 | -1.4023003 | -2.6236117 |

**2$(AuCl)_2$c**

Energy = -2765.784952808

| | | | |
|---|---|---|---|
| C | -1.8229328 | 1.5302889 | -3.2529663 |
| C | -1.1060137 | 2.0847725 | -2.1842392 |
| C | -1.2862769 | 3.4478667 | -1.8170652 |
| C | -2.1899960 | 4.2564215 | -2.5211775 |
| C | -2.9047438 | 3.6962814 | -3.5964552 |
| C | -2.7232685 | 2.3483464 | -3.9594868 |
| C | -0.1220915 | 1.4531815 | -1.2428111 |
| C | 0.3074779 | 2.5617516 | -0.3264886 |
| C | -0.4070100 | 3.7450557 | -0.6743101 |
| C | -0.1819281 | 4.9401352 | 0.0232072 |
| C | 0.7728496 | 4.9540783 | 1.0569234 |
| C | 1.5014407 | 3.7941866 | 1.3782031 |
| C | 1.2793497 | 2.5907322 | 0.6837184 |
| C | 0.0577094 | 0.0501730 | -1.1182291 |
| Au | 1.6613611 | 0.7170436 | -2.3342953 |
| Cl | 3.5486705 | 0.8151272 | -3.6228098 |
| P | 0.1320415 | -1.2815710 | 0.1435120 |
| C | -1.4692199 | -1.5646982 | 1.0314203 |
| C | -2.6412396 | -0.8609994 | 0.6820090 |
| C | -3.8208385 | -1.0582808 | 1.4166143 |
| C | -3.8466778 | -1.9688172 | 2.4851450 |
| C | -2.6792118 | -2.6642217 | 2.8396082 |
| C | -1.4868680 | -2.4512172 | 2.1305989 |
| C | 1.0518581 | -2.7900467 | -0.3962612 |
| C | 2.2378313 | -2.6584593 | -1.1538353 |
| C | 2.9600740 | -3.8019246 | -1.5267524 |
| C | 2.5147490 | -5.0778699 | -1.1455719 |
| C | 1.3330437 | -5.2090203 | -0.3986933 |
| C | 0.5978988 | -4.0745805 | -0.0249052 |
| C | 1.1558314 | -0.7646452 | 1.6538439 |
| C | 2.5297025 | -1.0689637 | 1.7673537 |
| C | 3.2817281 | -0.5906742 | 2.8544361 |
| C | 2.6723126 | 0.1923838 | 3.8475370 |
| C | 1.3053798 | 0.5007639 | 3.7454362 |
| C | 0.5547518 | 0.0304322 | 2.6570808 |
| Au | -1.0457969 | -1.7064640 | -1.9090139 |
| Cl | -2.2356769 | -3.5229573 | -2.7279411 |
| H | -1.6798536 | 0.4765236 | -3.5331053 |
| H | -3.2873656 | 1.9292973 | -4.8039099 |
| H | -3.6139439 | 4.3191260 | -4.1595830 |
| H | -2.3423881 | 5.3082158 | -2.2413859 |
| H | -0.7303478 | 5.8559442 | -0.2379726 |
| H | 0.9635759 | 5.8859688 | 1.6075945 |
| H | 2.2606364 | 3.8275891 | 2.1713751 |
| H | 1.8754132 | 1.7000709 | 0.9153175 |
| H | -2.6379541 | -0.1638855 | -0.1668618 |
| H | -0.5688008 | -2.9614667 | 2.4511313 |
| H | -2.6893697 | -3.3691421 | 3.6824313 |
| H | -4.7768025 | -2.1326234 | 3.0468716 |
| H | -4.7267238 | -0.5016051 | 1.1407000 |
| H | 0.8175443 | 1.1128722 | 4.5170167 |
| H | 3.2598463 | 0.5580948 | 4.7013909 |

| | | | |
|---|---|---|---|
| H | 4.3491219 | -0.8425053 | 2.9266435 |
| H | 3.0239364 | -1.6943949 | 1.0129677 |
| H | -0.5107785 | 0.2892820 | 2.5929440 |
| H | 3.8729487 | -3.6867058 | -2.1269917 |
| H | 3.0808440 | -5.9712799 | -1.4432596 |
| H | 0.9645279 | -6.2048473 | -0.1167120 |
| H | -0.3473482 | -4.1998301 | 0.5173973 |
| H | 2.5888152 | -1.6680333 | -1.4789527 |

**2($H^+$)**

Energy = -1574.112645037

| | | | |
|---|---|---|---|
| P | -0.2010296 | -1.1154775 | 0.4046862 |
| C | 0.7273939 | 2.1621701 | -0.7273123 |
| C | -0.5285048 | 1.4127562 | -0.9846304 |
| C | -1.3828119 | 2.3165468 | -1.8011090 |
| C | -2.6674981 | 2.1232060 | -2.3281783 |
| H | -3.2167668 | 1.1835467 | -2.1733309 |
| C | -3.2591660 | 3.1619338 | -3.0707446 |
| H | -4.2644636 | 3.0267478 | -3.4914145 |
| C | -2.5729415 | 4.3725794 | -3.2782363 |
| H | -3.0506659 | 5.1721671 | -3.8606895 |
| C | -1.2821263 | 4.5741907 | -2.7495429 |
| H | -0.7582438 | 5.5249646 | -2.9171566 |
| C | -0.6911630 | 3.5420373 | -2.0120019 |
| C | 0.6219138 | 3.4464751 | -1.3467991 |
| C | 1.6728134 | 4.3663266 | -1.2690225 |
| H | 1.5951480 | 5.3532310 | -1.7448116 |
| C | 2.8424359 | 4.0047950 | -0.5713510 |
| H | 3.6756804 | 4.7175814 | -0.5028841 |
| C | 2.9576460 | 2.7412292 | 0.0332952 |
| H | 3.8782280 | 2.4742775 | 0.5690969 |
| C | 1.9029068 | 1.8123038 | -0.0423852 |
| H | 2.0209383 | 0.8332856 | 0.4365480 |
| C | -0.9496090 | 0.1600176 | -0.6114304 |
| C | -2.0631228 | -3.0459916 | -0.3615319 |
| C | -1.5283949 | -2.3248598 | 0.7311611 |
| C | -2.0282457 | -2.5325634 | 2.0334616 |
| C | -3.0655114 | -3.4574604 | 2.2377162 |
| C | -3.6023697 | -4.1684932 | 1.1527710 |
| C | -3.1010907 | -3.9630731 | -0.1450912 |
| H | -1.6664182 | -2.9031059 | -1.3771443 |
| H | -1.6119788 | -1.9790854 | 2.8855533 |
| H | -3.4540453 | -3.6212485 | 3.2518387 |
| H | -4.4138351 | -4.8903183 | 1.3178797 |
| H | -3.5165837 | -4.5243375 | -0.9928587 |
| H | -0.5075546 | 1.8583743 | 4.3597961 |
| C | 0.0617975 | 1.0530992 | 3.8764313 |
| H | 1.5116000 | 0.8946684 | 5.4872024 |
| C | 1.1953791 | 0.5120674 | 4.5071780 |
| H | 2.8179234 | -0.9308461 | 4.3755702 |
| C | 1.9289615 | -0.5120477 | 3.8850319 |
| H | 2.1188388 | -1.7943388 | 2.1449132 |

| | | | |
|---|---|---|---|
| C | 1.5329465 | -1.0026225 | 2.6309695 |
| C | 0.3929302 | -0.4597097 | 1.9992469 |
| C | -0.3439320 | 0.5726040 | 2.6226217 |
| H | -1.2241756 | 1.0058591 | 2.1276691 |
| H | 3.2981735 | -1.6628807 | -3.1067000 |
| C | 2.7989216 | -2.1169144 | -2.2402742 |
| H | 3.9752523 | -3.9416547 | -2.3163650 |
| C | 3.1764654 | -3.3950636 | -1.7967735 |
| H | 2.8108704 | -4.9891592 | -0.3611832 |
| C | 2.5256734 | -3.9834548 | -0.6982272 |
| H | 0.9754877 | -3.7717229 | 0.8042120 |
| C | 1.4989062 | -3.2944552 | -0.0362949 |
| C | 1.1304843 | -2.0007167 | -0.4740978 |
| C | 1.7755667 | -1.4149371 | -1.5843177 |
| H | 1.4752434 | -0.4219867 | -1.9438167 |
| H | -1.9442973 | -0.1603063 | -0.9568929 |

**$2(H^+)_2$**

Energy = -1574.368601980

| | | | |
|---|---|---|---|
| P | -0.4038441 | -0.9951351 | 0.6631310 |
| C | 0.1948777 | 2.7041392 | -0.0858684 |
| C | -0.6337918 | 1.6392218 | -0.5990497 |
| C | -0.7256853 | 1.7840183 | -2.0321011 |
| C | -1.4336059 | 1.0233593 | -2.9912360 |
| H | -2.0293097 | 0.1467245 | -2.7025396 |
| C | -1.3716315 | 1.4124548 | -4.3409933 |
| H | -1.9152919 | 0.8411641 | -5.1042487 |
| C | -0.6226295 | 2.5416378 | -4.7149620 |
| H | -0.5907344 | 2.8399528 | -5.7722860 |
| C | 0.0922943 | 3.3202405 | -3.7565923 |
| H | 0.6591328 | 4.2016319 | -4.0849436 |
| C | 0.0374958 | 2.9383305 | -2.4249831 |
| C | 0.6226990 | 3.5206779 | -1.1915017 |
| C | 1.4169503 | 4.6351412 | -0.9714008 |
| H | 1.7520379 | 5.2805592 | -1.7942803 |
| C | 1.7933011 | 4.9458097 | 0.3696551 |
| H | 2.4176720 | 5.8311816 | 0.5545742 |
| C | 1.3790114 | 4.1563038 | 1.4554660 |
| H | 1.6808798 | 4.4295437 | 2.4745956 |
| C | 0.5691464 | 3.0264526 | 1.2394691 |
| H | 0.2395770 | 2.4150703 | 2.0903837 |
| C | -1.3311748 | 0.5992968 | 0.1987372 |
| C | -2.8463727 | -2.3469018 | 0.3335953 |
| C | -1.7047607 | -2.1591629 | 1.1509537 |
| C | -1.5356002 | -2.9348571 | 2.3229152 |
| C | -2.5114195 | -3.8804913 | 2.6733738 |
| C | -3.6490960 | -4.0560025 | 1.8688139 |
| C | -3.8144175 | -3.2918769 | 0.6988591 |
| H | -2.9899545 | -1.7745408 | -0.5939505 |
| H | -0.6492630 | -2.8077530 | 2.9577200 |
| H | -2.3798250 | -4.4815437 | 3.5828869 |
| H | -4.4127518 | -4.7928192 | 2.1522508 |

| | | | |
|---|---|---|---|
| H | -4.7018225 | -3.4337650 | 0.0678763 |
| H | 0.4617833 | 0.5436453 | 5.2916522 |
| C | 0.9053621 | 0.1247575 | 4.3783178 |
| H | 2.8958195 | -0.0505054 | 5.2354213 |
| C | 2.2718418 | -0.2133157 | 4.3461150 |
| H | 3.8987613 | -1.0468463 | 3.1684159 |
| C | 2.8361750 | -0.7702514 | 3.1869961 |
| H | 2.4897010 | -1.4441896 | 1.1541756 |
| C | 2.0439673 | -0.9896095 | 2.0484069 |
| C | 0.6740916 | -0.6412057 | 2.0758192 |
| C | 0.1020516 | -0.0876315 | 3.2498047 |
| H | -0.9706692 | 0.1514183 | 3.3039087 |
| H | 3.1263298 | -0.7107523 | -2.8173784 |
| C | 2.3204707 | -1.3189295 | -2.3851375 |
| H | 2.6587033 | -2.9971158 | -3.7245755 |
| C | 2.0580221 | -2.6053460 | -2.8924566 |
| H | 0.8389682 | -4.3986577 | -2.7271223 |
| C | 1.0371165 | -3.3922351 | -2.3350230 |
| H | -0.5158464 | -3.5288630 | -0.8252851 |
| C | 0.2704030 | -2.9021331 | -1.2662697 |
| C | 0.5313344 | -1.6076351 | -0.7584655 |
| C | 1.5616693 | -0.8138643 | -1.3208022 |
| H | 1.7900901 | 0.1843878 | -0.9209765 |
| H | -2.2276571 | 0.2367767 | -0.3365096 |
| H | -1.6603425 | 1.0001486 | 1.1768686 |

**3**

Energy = -763.9820254263

| | | | |
|---|---|---|---|
| C | -0.3599648 | -0.1917938 | 0.3183415 |
| C | -0.0231030 | -1.5153246 | 0.9087618 |
| C | -0.7580660 | -2.3124613 | 1.7961437 |
| H | -1.7404062 | -1.9669226 | 2.1493436 |
| C | -0.2147730 | -3.5408940 | 2.2132751 |
| H | -0.7769606 | -4.1799270 | 2.9094617 |
| C | 1.0473567 | -3.9636565 | 1.7471226 |
| H | 1.4553989 | -4.9272285 | 2.0846506 |
| C | 1.7903497 | -3.1679198 | 0.8559909 |
| H | 2.7733466 | -3.5069292 | 0.4985274 |
| C | 1.2522435 | -1.9400859 | 0.4362991 |
| C | 1.7729131 | -0.9019898 | -0.4717427 |
| C | 2.9709738 | -0.8194420 | -1.2000857 |
| H | 3.7184795 | -1.6242443 | -1.1490598 |
| C | 3.2040216 | 0.3134230 | -2.0011131 |
| H | 4.1378561 | 0.3904136 | -2.5762825 |
| C | 2.2538254 | 1.3514064 | -2.0746801 |
| H | 2.4553313 | 2.2283725 | -2.7065917 |
| C | 1.0516204 | 1.2743054 | -1.3471201 |
| H | 0.3100469 | 2.0843984 | -1.4043442 |
| C | 0.8109075 | 0.1493014 | -0.5467311 |
| C | -1.4891805 | 0.5115561 | 0.5430441 |
| N | -2.0354211 | 2.9216350 | 0.8419762 |
| N | -2.9928171 | 1.9208529 | -0.8531976 |

| | | | |
|---|---|---|---|
| C | -2.0674076 | 1.7031766 | 0.1659766 |
| C | -2.9380310 | 3.8299001 | 0.2832916 |
| C | -3.5349070 | 3.2060568 | -0.7734583 |
| H | -4.2909041 | 3.5648109 | -1.4740149 |
| H | -1.4569198 | 3.0745969 | 1.6630237 |
| H | -3.0737647 | 4.8370450 | 0.6811129 |
| H | -3.2520547 | 1.1975583 | -1.5179114 |

**3(AuCl)**

Energy = -1360.096313099

| | | | |
|---|---|---|---|
| C | -0.3935241 | -0.3419801 | 0.0926039 |
| C | 0.0984422 | -1.5717878 | 0.7562543 |
| C | -0.5424537 | -2.4669617 | 1.6304417 |
| H | -1.6093393 | -2.3398223 | 1.8690401 |
| C | 0.1926920 | -3.5291821 | 2.1838819 |
| H | -0.3079795 | -4.2376303 | 2.8582915 |
| C | 1.5589081 | -3.6967668 | 1.8839396 |
| H | 2.1162897 | -4.5326334 | 2.3298411 |
| C | 2.2152273 | -2.8035738 | 1.0179389 |
| H | 3.2824773 | -2.9347899 | 0.7896233 |
| C | 1.4830355 | -1.7490528 | 0.4537453 |
| C | 1.8856337 | -0.6965639 | -0.4867991 |
| C | 3.1008840 | -0.4859077 | -1.1557425 |
| H | 3.9676495 | -1.1316528 | -0.9561967 |
| C | 3.1892719 | 0.5432646 | -2.1089937 |
| H | 4.1345055 | 0.7155475 | -2.6425811 |
| C | 2.0609977 | 1.3285836 | -2.4128832 |
| H | 2.1253846 | 2.0958197 | -3.1972937 |
| C | 0.8418158 | 1.1252719 | -1.7413146 |
| H | -0.0343632 | 1.7146609 | -2.0429093 |
| C | 0.7521089 | 0.1421758 | -0.7345005 |
| C | -1.6543464 | 0.2178313 | 0.2710612 |
| N | -1.0335582 | 2.6815314 | 0.1177812 |
| N | -3.1039919 | 2.1841718 | -0.2538932 |
| C | -1.8881775 | 1.6184371 | 0.0059508 |
| C | -1.6986836 | 3.8794678 | -0.0802628 |
| C | -3.0158691 | 3.5609206 | -0.3148929 |
| H | -3.8808697 | 4.1991375 | -0.5034673 |
| H | -0.0338176 | 2.5590810 | 0.2902708 |
| H | -1.1969292 | 4.8474513 | -0.0254792 |
| H | -3.9429410 | 1.5904853 | -0.2826659 |
| Cl | -5.3303469 | -1.7600479 | 1.4811861 |
| Au | -3.3381527 | -0.7254855 | 0.9080238 |

**3$(AuCl)_2$a**

Energy = -1956.162765075

| | | | |
|---|---|---|---|
| C | -0.2305595 | -0.3365871 | 0.1304328 |
| C | 0.2790348 | -1.5801634 | 0.7481291 |
| C | -0.3344003 | -2.5133712 | 1.6036824 |
| H | -1.3876127 | -2.4025093 | 1.8983944 |
| C | 0.4155910 | -3.6019245 | 2.0798589 |
| H | -0.0622123 | -4.3357324 | 2.7430540 |

| | | | |
|---|---|---|---|
| C | 1.7669780 | -3.7618841 | 1.7170911 |
| H | 2.3368293 | -4.6180706 | 2.1043946 |
| C | 2.3927505 | -2.8374434 | 0.8608709 |
| H | 3.4470322 | -2.9672876 | 0.5789531 |
| C | 1.6463770 | -1.7558615 | 0.3741714 |
| C | 2.0136853 | -0.6729544 | -0.5471443 |
| C | 3.2049327 | -0.4310408 | -1.2446017 |
| H | 4.0796091 | -1.0805962 | -1.1007135 |
| C | 3.2608288 | 0.6418084 | -2.1524959 |
| H | 4.1880048 | 0.8398641 | -2.7081840 |
| C | 2.1262610 | 1.4440088 | -2.3781921 |
| H | 2.1696567 | 2.2525354 | -3.1211183 |
| C | 0.9299342 | 1.2104779 | -1.6772168 |
| H | 0.0519664 | 1.8258229 | -1.9127561 |
| C | 0.8711543 | 0.1722412 | -0.7255093 |
| C | -1.5048676 | 0.2257666 | 0.3344711 |
| N | -0.9976919 | 2.7083747 | 0.3104128 |
| N | -2.8092340 | 2.1245273 | -0.7111905 |
| C | -1.7397835 | 1.6235144 | -0.0416526 |
| C | -1.5953175 | 3.8776161 | -0.1303352 |
| C | -2.7491726 | 3.5060078 | -0.7779256 |
| H | -3.5200487 | 4.1052818 | -1.2653522 |
| H | -0.1284665 | 2.6285459 | 0.8405533 |
| H | -1.1671069 | 4.8637930 | 0.0579209 |
| H | -3.5528451 | 1.5013581 | -1.0501714 |
| Cl | -4.7397915 | -2.1744159 | -1.3773445 |
| Au | -3.1764943 | -1.0170968 | -0.1526965 |
| Cl | -3.0106708 | 0.4303225 | 4.4515363 |
| Au | -2.4742207 | 0.1051223 | 2.2407835 |

**3$(AuCl)_2$b**

Energy = -1956.160486511

| | | | |
|---|---|---|---|
| C | -2.6549724 | 3.4672081 | -0.6350676 |
| N | -2.7143744 | 2.0828790 | -0.5755249 |
| C | -1.6448935 | 1.5809922 | 0.0982029 |
| N | -0.8980778 | 2.6650051 | 0.4438367 |
| C | -1.5032905 | 3.8383905 | 0.0111664 |
| C | -1.4144730 | 0.1979653 | 0.5075136 |
| Au | -2.6473625 | -0.1404023 | 2.1001011 |
| Cl | -4.0335964 | -0.4775799 | 3.9130889 |
| C | -0.2106213 | -0.4828896 | 0.1412739 |
| C | 0.4151526 | -1.6142203 | 0.8913282 |
| C | 1.7628243 | -1.7656620 | 0.4542358 |
| C | 2.0302986 | -0.7731705 | -0.5976496 |
| C | 0.8465731 | -0.0077904 | -0.8115143 |
| C | 2.5923259 | -2.7420390 | 1.0248952 |
| C | 2.0674135 | -3.5722064 | 2.0313656 |
| C | 0.7354835 | -3.4239836 | 2.4632448 |
| C | -0.0996152 | -2.4439078 | 1.8989805 |
| C | 0.8150915 | 0.9710787 | -1.8186386 |
| C | 1.9746416 | 1.2126890 | -2.5774814 |
| C | 3.1502658 | 0.4746179 | -2.3437139 |

| | | | |
|---|---|---|---|
| C | 3.1834977 | -0.5280791 | -1.3585428 |
| Au | -2.0333022 | -1.2351264 | -0.9877883 |
| Cl | -3.3155435 | -2.3732643 | -2.4990749 |
| H | -1.1388377 | -2.3282812 | 2.2411130 |
| H | 0.3400028 | -4.0810862 | 3.2497279 |
| H | 2.7036338 | -4.3444025 | 2.4862052 |
| H | 3.6343818 | -2.8586040 | 0.6957914 |
| H | 4.0977708 | -1.1159269 | -1.1968692 |
| H | 4.0456261 | 0.6728655 | -2.9494118 |
| H | 1.9564612 | 1.9733251 | -3.3701818 |
| H | -0.1058926 | 1.5240763 | -2.0491796 |
| H | -3.4246255 | 4.0665838 | -1.1240946 |
| H | -0.0282349 | 2.5891325 | 0.9716837 |
| H | -1.0737703 | 4.8239599 | 0.1981231 |
| H | -3.4554760 | 1.4767275 | -0.9362456 |

**3$(AuCl)_2$c**

Energy = -1956.137323518

| | | | |
|---|---|---|---|
| N | -0.8791394 | 2.7533711 | 0.5816814 |
| C | -1.6585323 | 1.6409120 | 0.3103068 |
| N | -2.7248429 | 2.1481533 | -0.4144212 |
| C | -2.6942200 | 3.5394713 | -0.4277956 |
| C | -1.5427128 | 3.9200302 | 0.2030940 |
| C | -1.2540381 | 0.2460181 | 0.4479185 |
| Au | -2.4223339 | 0.6751409 | 2.1815203 |
| Cl | -3.6814302 | 1.1376081 | 4.0498626 |
| C | -0.0825386 | -0.4618751 | 0.0913414 |
| C | 0.9551828 | -0.0473422 | -0.9042095 |
| C | 2.1068595 | -0.8683731 | -0.7302671 |
| C | 1.8439159 | -1.8196007 | 0.3646724 |
| C | 0.5332191 | -1.5803688 | 0.8668154 |
| C | 0.9260984 | 0.9479327 | -1.8919270 |
| C | 2.0613969 | 1.1309958 | -2.7025821 |
| C | 3.2032444 | 0.3263734 | -2.5266203 |
| C | 3.2335598 | -0.6812588 | -1.5445956 |
| C | 2.6498922 | -2.8107212 | 0.9431815 |
| C | 2.1357111 | -3.5574763 | 2.0195879 |
| C | 0.8387679 | -3.3173549 | 2.5133733 |
| C | 0.0269477 | -2.3207031 | 1.9435226 |
| Au | -1.9222566 | -1.2445433 | -0.9039189 |
| Cl | -3.2489795 | -2.5109257 | -2.2648369 |
| H | -0.9849564 | -2.1261457 | 2.3262317 |
| H | 0.4598219 | -3.9076475 | 3.3588291 |
| H | 2.7513649 | -4.3455604 | 2.4753701 |
| H | 3.6699970 | -2.9942562 | 0.5779112 |
| H | 4.1295790 | -1.3050813 | -1.4193928 |
| H | 4.0779517 | 0.4783688 | -3.1745601 |
| H | 2.0560691 | 1.9061955 | -3.4812443 |
| H | 0.0276878 | 1.5604948 | -2.0499931 |
| H | -3.4942837 | 4.1351047 | -0.8700827 |
| H | -0.0234187 | 2.7015274 | 1.1309122 |
| H | -1.1447923 | 4.9126887 | 0.4205221 |

| | | | |
|---|---|---|---|
| H | -3.4693515 | 1.5504545 | -0.7725934 |

**3($H^+$)**

Energy = -764.4331488940

| | | | |
|---|---|---|---|
| C | -0.0376452 | -0.0117653 | 0.4061237 |
| C | 0.2801870 | -1.3498273 | 0.9496361 |
| C | -0.3283874 | -2.0864355 | 1.9784822 |
| H | -1.1574239 | -1.6733959 | 2.5706155 |
| C | 0.1475825 | -3.3801234 | 2.2584980 |
| H | -0.3104293 | -3.9659398 | 3.0662698 |
| C | 1.2053294 | -3.9299746 | 1.5108003 |
| H | 1.5605624 | -4.9435083 | 1.7411307 |
| C | 1.8164808 | -3.1996072 | 0.4701299 |
| H | 2.6377028 | -3.6440760 | -0.1079111 |
| C | 1.3545350 | -1.9080421 | 0.1985173 |
| C | 1.7980666 | -0.8994125 | -0.7821557 |
| C | 2.8556030 | -0.9234534 | -1.6972819 |
| H | 3.4764326 | -1.8213107 | -1.8170879 |
| C | 3.1337230 | 0.2352227 | -2.4496804 |
| H | 3.9630188 | 0.2293894 | -3.1698898 |
| C | 2.3855788 | 1.4100640 | -2.2605035 |
| H | 2.6490365 | 2.3204800 | -2.8150121 |
| C | 1.3144996 | 1.4360036 | -1.3470632 |
| H | 0.8055953 | 2.3920180 | -1.1645712 |
| C | 0.9837126 | 0.2678411 | -0.6329128 |
| C | -1.1399673 | 0.7065615 | 0.8283421 |
| N | -2.7576759 | 2.5865870 | 0.8394073 |
| N | -1.6927227 | 2.3388045 | -1.0287812 |
| C | -1.7876953 | 1.8366369 | 0.2353776 |
| C | -3.2579935 | 3.5413446 | -0.0291487 |
| C | -2.5837858 | 3.3820444 | -1.2150951 |
| H | -2.6679208 | 3.9205182 | -2.1613885 |
| H | -3.0504052 | 2.4566545 | 1.8093193 |
| H | -4.0377250 | 4.2492501 | 0.2594753 |
| H | -1.0730947 | 1.9394398 | -1.7396103 |
| H | -1.6733460 | 0.3194914 | 1.7090197 |

**3($H^+$)$_2$**

Energy = -764.6594821589

| | | | |
|---|---|---|---|
| C | -0.2305993 | -0.3798986 | -0.1927698 |
| C | 0.1976840 | -1.4589538 | 0.6498024 |
| C | -0.5233495 | -2.2506102 | 1.5818336 |
| H | -1.5946502 | -2.0914567 | 1.7705486 |
| C | 0.1588670 | -3.2671743 | 2.2707246 |
| H | -0.3749973 | -3.8972670 | 2.9935439 |
| C | 1.5289439 | -3.4811801 | 2.0333099 |
| H | 2.0499880 | -4.2801147 | 2.5797714 |
| C | 2.2684064 | -2.6903716 | 1.0974786 |
| H | 3.3360038 | -2.8935555 | 0.9398741 |
| C | 1.6018576 | -1.6892376 | 0.4126149 |
| C | 2.0389134 | -0.7139954 | -0.6192735 |
| C | 3.2553369 | -0.5031352 | -1.2479270 |

| | | | |
|---|---|---|---|
| H | 4.1456193 | -1.0985845 | -1.0056610 |
| C | 3.3364003 | 0.5152068 | -2.2470158 |
| H | 4.2974088 | 0.6894002 | -2.7511981 |
| C | 2.2201842 | 1.2918819 | -2.6059714 |
| H | 2.3171542 | 2.0580177 | -3.3858001 |
| C | 0.9835205 | 1.0817897 | -1.9715383 |
| H | 0.1128510 | 1.6843682 | -2.2661102 |
| C | 0.8900402 | 0.0810183 | -0.9730528 |
| C | -1.6567772 | 0.1085288 | -0.2837600 |
| N | -1.3313009 | 2.4467246 | 0.7128215 |
| N | -2.7657511 | 2.3211112 | -0.8940099 |
| C | -1.8779793 | 1.5911260 | -0.1808120 |
| C | -1.8678029 | 3.7157409 | 0.5665254 |
| C | -2.7842546 | 3.6347559 | -0.4554195 |
| H | -3.4355375 | 4.3945971 | -0.8962121 |
| H | -0.6240659 | 2.1894945 | 1.4077880 |
| H | -1.5617386 | 4.5610767 | 1.1888350 |
| H | -3.3626228 | 1.9466969 | -1.6388208 |
| H | -2.0668032 | -0.2330578 | -1.2588053 |
| H | -2.2776813 | -0.3913335 | 0.4872869 |

**4**

Energy = -996.1074717574

| | | | |
|---|---|---|---|
| C | 0.6700650 | -1.1651294 | 0.3079137 |
| C | 0.9449174 | -2.4903367 | 0.9285221 |
| C | 0.1639530 | -3.2459620 | 1.8123974 |
| H | -0.8133455 | -2.8641836 | 2.1415263 |
| C | 0.6554900 | -4.4856377 | 2.2600872 |
| H | 0.0569122 | -5.0929540 | 2.9540098 |
| C | 1.9109552 | -4.9586389 | 1.8271197 |
| H | 2.2782193 | -5.9299905 | 2.1880826 |
| C | 2.6997672 | -4.2038296 | 0.9392847 |
| H | 3.6773578 | -4.5825331 | 0.6080991 |
| C | 2.2140169 | -2.9656194 | 0.4891516 |
| C | 2.7900123 | -1.9616746 | -0.4245698 |
| C | 4.0041328 | -1.9322835 | -1.1290848 |
| H | 4.7225248 | -2.7608861 | -1.0504729 |
| C | 4.2912937 | -0.8207800 | -1.9428929 |
| H | 5.2384327 | -0.7853968 | -2.4999276 |
| C | 3.3797307 | 0.2479572 | -2.0530183 |
| H | 3.6238376 | 1.1066940 | -2.6944868 |
| C | 2.1613173 | 0.2241414 | -1.3492962 |
| H | 1.4472555 | 1.0566382 | -1.4329194 |
| C | 1.8689837 | -0.8790887 | -0.5374739 |
| C | -0.4266108 | -0.4098086 | 0.4853673 |
| N | -1.1129492 | 1.9175489 | 0.9504621 |
| N | -2.0888539 | 0.8985382 | -0.7912594 |
| C | -1.1078531 | 0.7347869 | 0.1972477 |
| C | -2.0580423 | 2.8018613 | 0.4358412 |
| C | -2.6775265 | 2.1549945 | -0.6697319 |
| C | -4.0531709 | 4.0960986 | -1.0229371 |
| C | -0.2505832 | 2.1381642 | 2.0900300 |

| | | | |
|---|---|---|---|
| C | -3.4416760 | 4.7346313 | 0.0687134 |
| C | -2.4109341 | -0.1177383 | -1.7681630 |
| C | -3.6760491 | 2.7919208 | -1.4144519 |
| C | -2.4263572 | 4.0968019 | 0.8161843 |
| H | -4.8339998 | 4.6198699 | -1.5910208 |
| H | -0.7733217 | 2.7616087 | 2.8385264 |
| H | -3.7496068 | 5.7522412 | 0.3451419 |
| H | -1.8293301 | -0.0006696 | -2.7055104 |
| H | -4.1473893 | 2.3024418 | -2.2766403 |
| H | -1.9420470 | 4.6052685 | 1.6600052 |
| H | -3.4890996 | -0.0757240 | -2.0090661 |
| H | -2.1801549 | -1.1092750 | -1.3356537 |
| H | 0.6998333 | 2.6365760 | 1.8091550 |
| H | -0.0101072 | 1.1593567 | 2.5457188 |

**4(AuCl)**

Energy = -1592.213557488

| | | | |
|---|---|---|---|
| C | -2.4759288 | 3.6598446 | 1.2523306 |
| C | -2.0721005 | 2.3734751 | 0.8673009 |
| C | -2.7479331 | 1.6609096 | -0.1559123 |
| C | -3.8492504 | 2.2116716 | -0.8266495 |
| C | -4.2549901 | 3.4985416 | -0.4367938 |
| C | -3.5817692 | 4.2083821 | 0.5823030 |
| N | -2.0939763 | 0.4354097 | -0.2879986 |
| C | -1.0585421 | 0.3750208 | 0.6066515 |
| N | -1.0376307 | 1.5491681 | 1.3116836 |
| C | -0.0965040 | 1.8467840 | 2.3821943 |
| C | -2.4592975 | -0.6429386 | -1.1956005 |
| C | -0.2071026 | -0.7763035 | 0.8449482 |
| C | 0.9793083 | -0.9773606 | 0.1777573 |
| C | 1.9060262 | -2.1238688 | 0.3481204 |
| C | 3.0200989 | -1.9582499 | -0.5278511 |
| C | 2.8365420 | -0.7068828 | -1.2768485 |
| C | 1.6078629 | -0.1077068 | -0.8581428 |
| C | 4.0501831 | -2.9104580 | -0.5663463 |
| C | 3.9655767 | -4.0339323 | 0.2753686 |
| C | 2.8668318 | -4.2005416 | 1.1413725 |
| C | 1.8321431 | -3.2492759 | 1.1836879 |
| C | 1.2039281 | 1.1110762 | -1.4318591 |
| C | 2.0134608 | 1.7206286 | -2.4085641 |
| C | 3.2212444 | 1.1235860 | -2.8155220 |
| C | 3.6395403 | -0.0943889 | -2.2510185 |
| H | 0.9743763 | -3.3811624 | 1.8608985 |
| H | 2.8154753 | -5.0840207 | 1.7928456 |
| H | 4.7639641 | -4.7893796 | 0.2575032 |
| H | 4.9094410 | -2.7851794 | -1.2405089 |
| H | 4.5836607 | -0.5577340 | -2.5707345 |
| H | 3.8412094 | 1.6136154 | -3.5794992 |
| H | 1.6976178 | 2.6732255 | -2.8568901 |
| H | 0.2684308 | 1.6044530 | -1.1367145 |
| H | -5.1143672 | 3.9633237 | -0.9381577 |
| H | -0.6209469 | 2.3925890 | 3.1858877 |

| | | | |
|---|---|---|---|
| H | -3.9286575 | 5.2135270 | 0.8566987 |
| H | -2.0476206 | -0.4673284 | -2.2072084 |
| H | -4.3716334 | 1.6654815 | -1.6220047 |
| H | -1.9528770 | 4.2166747 | 2.0398642 |
| H | -3.5596753 | -0.7160253 | -1.2497591 |
| H | -2.0539502 | -1.5878813 | -0.7940022 |
| H | 0.7496691 | 2.4545131 | 2.0102916 |
| H | 0.2860663 | 0.8923659 | 2.7844346 |
| Au | -1.1357245 | -1.8802541 | 2.2621525 |
| Cl | -2.2084609 | -3.1315159 | 3.8898715 |

**4(AuCl)$_2$a**

Energy = -2188.271968067

| | | | |
|---|---|---|---|
| C | -2.9108996 | 3.4760095 | 1.1879180 |
| C | -2.2930017 | 2.2640047 | 0.8414128 |
| C | -2.5671101 | 1.6180140 | -0.3865873 |
| C | -3.4619486 | 2.1642370 | -1.3207810 |
| C | -4.0771256 | 3.3756878 | -0.9748072 |
| C | -3.8075651 | 4.0187984 | 0.2561712 |
| N | -1.8051204 | 0.4535873 | -0.4039148 |
| C | -1.0778954 | 0.3648280 | 0.7582528 |
| N | -1.3598868 | 1.4724788 | 1.5129926 |
| C | -0.7715446 | 1.8476801 | 2.7966281 |
| C | -1.7982932 | -0.4994215 | -1.5080311 |
| C | -0.2208457 | -0.7876003 | 1.1023935 |
| C | 0.9158538 | -1.0248237 | 0.3073527 |
| C | 1.7243905 | -2.2662370 | 0.2694261 |
| C | 2.7396856 | -2.1260340 | -0.7252991 |
| C | 2.6367254 | -0.7798872 | -1.3022021 |
| C | 1.5469926 | -0.1013781 | -0.6676194 |
| C | 3.6275299 | -3.1746022 | -1.0027520 |
| C | 3.5088624 | -4.3734977 | -0.2768650 |
| C | 2.5139100 | -4.5174780 | 0.7090837 |
| C | 1.6175216 | -3.4714010 | 0.9868550 |
| C | 1.2964877 | 1.2467121 | -0.9928064 |
| C | 2.0852330 | 1.8851212 | -1.9668971 |
| C | 3.1319418 | 1.1971881 | -2.6088657 |
| C | 3.4188935 | -0.1380937 | -2.2718924 |
| H | 0.8494659 | -3.6014684 | 1.7625470 |
| H | 2.4351205 | -5.4571699 | 1.2724742 |
| H | 4.1987980 | -5.2046278 | -0.4796838 |
| H | 4.4045873 | -3.0658775 | -1.7724323 |
| H | 4.2533956 | -0.6644290 | -2.7559447 |
| H | 3.7394235 | 1.7126042 | -3.3658889 |
| H | 1.8881283 | 2.9364437 | -2.2188910 |
| H | 0.5143988 | 1.8271881 | -0.4869446 |
| H | -4.7860642 | 3.8352290 | -1.6762626 |
| H | -1.4176124 | 1.5264782 | 3.6342098 |
| H | -4.3146255 | 4.9643024 | 0.4901342 |
| H | -1.1271696 | -0.1488440 | -2.3142037 |
| H | -3.6720060 | 1.6701199 | -2.2772465 |
| H | -2.7136397 | 3.9742190 | 2.1450383 |

| | | | |
|---|---|---|---|
| H | -2.8277872 | -0.6098284 | -1.8902745 |
| H | -1.4512985 | -1.4792324 | -1.1402236 |
| H | -0.6505206 | 2.9449331 | 2.8166561 |
| H | 0.2145570 | 1.3696289 | 2.9107591 |
| Au | 0.0583766 | -1.2349715 | 3.1772727 |
| Cl | 0.8066337 | -1.1555819 | 5.3558676 |
| Au | -1.6682792 | -2.3709770 | 1.4453049 |
| Cl | -3.3466834 | -3.8920409 | 1.0485765 |

**4$(AuCl)_2$b**

Energy = -2188.275761843

| | | | |
|---|---|---|---|
| C | 3.4355584 | -0.2192770 | -2.3979360 |
| C | 2.6706025 | -0.8420165 | -1.3996068 |
| C | 1.7584082 | -0.0827542 | -0.6106568 |
| C | 1.6446133 | 1.3040344 | -0.8015768 |
| C | 2.4105949 | 1.9213775 | -1.8069934 |
| C | 3.2938325 | 1.1649448 | -2.6009435 |
| C | 1.0843591 | -1.0009078 | 0.3658564 |
| C | 1.6954981 | -2.3456849 | 0.1257092 |
| C | 2.6290905 | -2.2406153 | -0.9463339 |
| C | 3.3238402 | -3.3715310 | -1.3999269 |
| C | 3.0868512 | -4.6086210 | -0.7744837 |
| C | 2.1658009 | -4.7131843 | 0.2850428 |
| C | 1.4628025 | -3.5845302 | 0.7418832 |
| C | -0.1169950 | -0.7352001 | 1.1049934 |
| Au | -1.2761913 | -2.0708395 | 2.1283247 |
| Cl | -2.5860169 | -3.5875332 | 3.2775871 |
| C | -0.9848682 | 0.3822347 | 0.7434580 |
| N | -1.5633074 | 0.5266132 | -0.4937688 |
| C | -2.4251210 | 1.6224572 | -0.4737951 |
| C | -2.3750115 | 2.1557347 | 0.8378074 |
| N | -1.4820369 | 1.3630463 | 1.5620491 |
| C | -3.2341274 | 2.1918102 | -1.4685849 |
| C | -3.9948463 | 3.3139728 | -1.1060599 |
| C | -3.9456929 | 3.8469721 | 0.2016190 |
| C | -3.1344081 | 3.2798424 | 1.1964600 |
| C | -1.3982874 | -0.3919201 | -1.6132992 |
| C | -1.2183732 | 1.4791670 | 2.9925926 |
| Au | 1.5502182 | -0.3303943 | 2.4401698 |
| Cl | 2.7707370 | 0.3070522 | 4.2669901 |
| H | 0.7441855 | -3.6699007 | 1.5705944 |
| H | 1.9932792 | -5.6860097 | 0.7651832 |
| H | 3.6263826 | -5.5030678 | -1.1162551 |
| H | 4.0402394 | -3.2972134 | -2.2300423 |
| H | 4.1417846 | -0.7995324 | -3.0079206 |
| H | 3.8903019 | 1.6650758 | -3.3767761 |
| H | 2.3304918 | 3.0061965 | -1.9615625 |
| H | 0.9945898 | 1.9152989 | -0.1604140 |
| H | -4.6391782 | 3.7895811 | -1.8573560 |
| H | -1.3407231 | 0.4853644 | 3.4646913 |
| H | -4.5542720 | 4.7274517 | 0.4469331 |
| H | -0.5774474 | -0.0684317 | -2.2795178 |

| | | | |
|---|---|---|---|
| H | -3.2685242 | 1.7859632 | -2.4873154 |
| H | -3.0994999 | 3.7037673 | 2.2076630 |
| H | -2.3452161 | -0.4328056 | -2.1788393 |
| H | -1.1766582 | -1.3997928 | -1.2224791 |
| H | -1.9494393 | 2.1792311 | 3.4277143 |
| H | -0.1923706 | 1.8427957 | 3.1854297 |

**4$(AuCl)_2$c**

Energy = -2188.2555600540

| | | | |
|---|---|---|---|
| C | 1.3426186 | -3.5210870 | 0.5232509 |
| C | 1.7138955 | -2.2809104 | -0.0136440 |
| C | 2.7493922 | -2.1838604 | -0.9867367 |
| C | 3.4227620 | -3.3369011 | -1.4154696 |
| C | 3.0542581 | -4.5795387 | -0.8667258 |
| C | 2.0246934 | -4.6720727 | 0.0896840 |
| C | 1.1547307 | -0.9162637 | 0.2290459 |
| C | 1.9253445 | -0.0024050 | -0.6673508 |
| C | 2.8810242 | -0.7723418 | -1.3919276 |
| C | 3.7322400 | -0.1460310 | -2.3140294 |
| C | 3.6221110 | 1.2442677 | -2.5050283 |
| C | 2.6787042 | 2.0025624 | -1.7858915 |
| C | 1.8245065 | 1.3834376 | -0.8548178 |
| C | -0.0498420 | -0.6144058 | 0.9071987 |
| Au | -1.8677355 | -1.6240875 | 1.4326616 |
| Cl | -3.8162889 | -2.7063612 | 1.9958554 |
| Au | 1.4634346 | -0.4247439 | 2.3752743 |
| Cl | 2.5708313 | -0.0524230 | 4.3399888 |
| C | -1.1469027 | 0.3068609 | 0.6613208 |
| N | -1.5900316 | 1.3599876 | 1.4658736 |
| C | -2.4739013 | 2.1578314 | 0.7380578 |
| C | -2.5231773 | 1.6365055 | -0.5805238 |
| N | -1.6668535 | 0.5372178 | -0.6154548 |
| C | -3.3301961 | 2.2248064 | -1.5628636 |
| C | -4.0831269 | 3.3545431 | -1.1913127 |
| C | -4.0327229 | 3.8723449 | 0.1177450 |
| C | -3.2243761 | 3.2811581 | 1.1069887 |
| C | -1.2890476 | 1.5246656 | 2.8787312 |
| C | -1.4677556 | -0.3729589 | -1.7294115 |
| H | 0.5364578 | -3.5879820 | 1.2675996 |
| H | 1.7497225 | -5.6527244 | 0.5014219 |
| H | 3.5743470 | -5.4913155 | -1.1923687 |
| H | 4.2186758 | -3.2788291 | -2.1710284 |
| H | 4.4741737 | -0.7256558 | -2.8807562 |
| H | 4.2853788 | 1.7462625 | -3.2233581 |
| H | 2.6155203 | 3.0876581 | -1.9458285 |
| H | 1.1057627 | 1.9798604 | -0.2760699 |
| H | -4.7252057 | 3.8378389 | -1.9398555 |
| H | -1.1575267 | 0.5336229 | 3.3486081 |
| H | -4.6281917 | 4.7589687 | 0.3729649 |
| H | -0.4857689 | -0.2241189 | -2.2170264 |
| H | -3.3712621 | 1.8320955 | -2.5867473 |
| H | -3.1848891 | 3.6909910 | 2.1239804 |

| | | | |
|---|---|---|---|
| H | -2.2668764 | -0.2132359 | -2.4724293 |
| H | -1.5333036 | -1.4154766 | -1.3579456 |
| H | -2.1385574 | 2.0298464 | 3.3699441 |
| H | -0.3672709 | 2.1173404 | 3.0371511 |

**4($H^+$)**

Energy = -996.5499372413

| | | | |
|---|---|---|---|
| C | -3.3381514 | 3.0554377 | 1.8020346 |
| C | -2.5653860 | 2.0292753 | 1.2348685 |
| C | -2.7006821 | 1.6624680 | -0.1264383 |
| C | -3.6154311 | 2.3063144 | -0.9756080 |
| C | -4.3866869 | 3.3287594 | -0.4077803 |
| C | -4.2503569 | 3.6961710 | 0.9533742 |
| N | -1.8032192 | 0.6163440 | -0.3544731 |
| C | -1.1179365 | 0.3564401 | 0.8023235 |
| N | -1.5786800 | 1.2025344 | 1.7733001 |
| C | -1.0859990 | 1.2691095 | 3.1463475 |
| C | -1.7303610 | -0.1457120 | -1.5975118 |
| C | -0.1643013 | -0.7085449 | 1.0329784 |
| C | 0.9369008 | -1.0449673 | 0.2779831 |
| C | 1.7175133 | -2.2866747 | 0.4801980 |
| C | 2.7597682 | -2.3374183 | -0.4901365 |
| C | 2.6955435 | -1.1028350 | -1.2963116 |
| C | 1.6018405 | -0.3118015 | -0.8260710 |
| C | 3.6275565 | -3.4335313 | -0.5427710 |
| C | 3.4517404 | -4.4789003 | 0.3868851 |
| C | 2.4237423 | -4.4311956 | 1.3466596 |
| C | 1.5437355 | -3.3344878 | 1.3969818 |
| C | 1.3835437 | 0.9703205 | -1.3593123 |
| C | 2.2192694 | 1.4358770 | -2.3920034 |
| C | 3.2680862 | 0.6346353 | -2.8775030 |
| C | 3.5205085 | -0.6374602 | -2.3260232 |
| H | 0.7406536 | -3.3144487 | 2.1476144 |
| H | 2.3064091 | -5.2574099 | 2.0603222 |
| H | 4.1265291 | -5.3453483 | 0.3605757 |
| H | 4.4313215 | -3.4875858 | -1.2893919 |
| H | 4.3617143 | -1.2411402 | -2.6924651 |
| H | 3.9106678 | 1.0130193 | -3.6841896 |
| H | 2.0577400 | 2.4368325 | -2.8139304 |
| H | 0.5934149 | 1.6273389 | -0.9711256 |
| H | -5.1148551 | 3.8604652 | -1.0341368 |
| H | -1.7943759 | 0.7788811 | 3.8401806 |
| H | -4.8776832 | 4.5031479 | 1.3540866 |
| H | -1.1566077 | 0.4064786 | -2.3644977 |
| H | -3.7216365 | 2.0316886 | -2.0322743 |
| H | -3.2427340 | 3.3421565 | 2.8565247 |
| H | -2.7557145 | -0.3309442 | -1.9627881 |
| H | -1.2311075 | -1.1083919 | -1.4047696 |
| H | -0.9650801 | 2.3266633 | 3.4394961 |
| H | -0.1048614 | 0.7709008 | 3.2061633 |
| H | -0.3763619 | -1.3224815 | 1.9226249 |

**$4(H^+)_2$**

Energy = -996.7868881385

| | | | |
|---|---|---|---|
| C | -3.1180453 | 3.3317490 | 1.2739486 |
| C | -2.4378085 | 2.1411674 | 0.9659375 |
| C | -2.7808253 | 1.3559361 | -0.1605268 |
| C | -3.8151541 | 1.7263495 | -1.0370438 |
| C | -4.4888127 | 2.9143442 | -0.7313733 |
| C | -4.1479711 | 3.6997776 | 0.4004705 |
| N | -1.9253382 | 0.2487576 | -0.1505856 |
| C | -1.0919733 | 0.3449527 | 0.9190590 |
| N | -1.3819009 | 1.4816325 | 1.6089942 |
| C | -0.7852006 | 1.9615641 | 2.8592413 |
| C | -1.9870845 | -0.8312325 | -1.1368915 |
| C | -0.0872617 | -0.6955985 | 1.3258154 |
| C | 1.0289502 | -1.0330128 | 0.3711754 |
| C | 1.6004464 | -2.3487592 | 0.2570610 |
| C | 2.7033916 | -2.2876106 | -0.6667618 |
| C | 2.8065311 | -0.8824003 | -1.1353467 |
| C | 1.7628686 | -0.1321635 | -0.4831523 |
| C | 3.4427685 | -3.4245213 | -0.9472603 |
| C | 3.0818395 | -4.6455691 | -0.2980529 |
| C | 2.0077306 | -4.7162326 | 0.6069613 |
| C | 1.2512678 | -3.5665949 | 0.8928374 |
| C | 1.6244253 | 1.2582259 | -0.7152486 |
| C | 2.5213302 | 1.8915354 | -1.5930439 |
| C | 3.5326297 | 1.1477383 | -2.2263734 |
| C | 3.6873974 | -0.2528671 | -2.0001655 |
| H | 0.4115132 | -3.6307907 | 1.5993778 |
| H | 1.7610384 | -5.6713825 | 1.0879903 |
| H | 3.6626523 | -5.5533264 | -0.5143440 |
| H | 4.2909328 | -3.4099956 | -1.6445996 |
| H | 4.4957078 | -0.7993783 | -2.5039331 |
| H | 4.2258882 | 1.6558319 | -2.9113826 |
| H | 2.4354942 | 2.9685183 | -1.7861494 |
| H | 0.8393297 | 1.8469202 | -0.2225038 |
| H | -5.3067370 | 3.2480210 | -1.3833349 |
| H | -1.4929924 | 1.8173656 | 3.6962261 |
| H | -4.7115816 | 4.6210846 | 0.5977405 |
| H | -1.7393413 | -0.4410110 | -2.1406773 |
| H | -4.0901277 | 1.1243543 | -1.9118809 |
| H | -2.8707281 | 3.9428600 | 2.1506182 |
| H | -3.0080543 | -1.2535685 | -1.1538642 |
| H | -1.2763085 | -1.6307388 | -0.8760114 |
| H | -0.5546467 | 3.0365684 | 2.7606803 |
| H | 0.1516023 | 1.4256215 | 3.0784046 |
| H | 0.3992045 | -0.3623286 | 2.2672938 |
| H | -0.6270568 | -1.6217836 | 1.6106845 |

**5**

Energy = -808.0518925608

| | | | |
|---|---|---|---|
| C | 12.7727384 | 1.3017806 | 1.8742592 |
| C | 11.3674616 | 0.8795269 | 1.6077345 |

| | | | |
|---|---|---|---|
| C | 10.3979521 | 0.3568979 | 2.4732755 |
| H | 10.6278978 | 0.2005344 | 3.5369806 |
| C | 9.1300617 | 0.0380721 | 1.9540963 |
| H | 8.3567478 | -0.3730792 | 2.6183531 |
| C | 8.8404850 | 0.2406070 | 0.5896578 |
| H | 7.8436074 | -0.0147678 | 0.2032391 |
| C | 9.8107833 | 0.7651162 | -0.2827110 |
| H | 9.5751895 | 0.9196242 | -1.3453376 |
| C | 11.0797895 | 1.0861315 | 0.2270851 |
| C | 12.2803060 | 1.6401423 | -0.4211455 |
| C | 12.5293589 | 2.0193849 | -1.7506142 |
| H | 11.7496170 | 1.9223276 | -2.5194936 |
| C | 13.7967398 | 2.5278658 | -2.0865046 |
| H | 14.0043758 | 2.8281452 | -3.1233366 |
| C | 14.8048813 | 2.6572938 | -1.1100368 |
| H | 15.7886053 | 3.0568948 | -1.3944812 |
| C | 14.5643674 | 2.2800350 | 0.2235887 |
| H | 15.3480097 | 2.3793953 | 0.9883476 |
| C | 13.3032717 | 1.7730080 | 0.5624812 |
| C | 13.4173665 | 1.2657079 | 3.0371073 |
| C | 14.0697035 | 1.2297245 | 4.2132751 |
| C | 13.9997478 | 2.4124043 | 5.0940402 |
| H | 13.3972975 | 3.2346073 | 4.6784593 |
| C | 14.5586406 | 2.6352361 | 6.3214064 |
| H | 14.3424566 | 3.6208450 | 6.7622814 |
| C | 15.3954767 | 1.7765456 | 7.1405045 |
| H | 15.7125810 | 2.2107555 | 8.1009932 |
| C | 15.8291967 | 0.5095139 | 6.8610726 |
| H | 16.4620160 | 0.0218003 | 7.6182293 |
| C | 15.5588202 | -0.2864488 | 5.6770182 |
| H | 16.0222802 | -1.2852850 | 5.6800724 |
| C | 14.8226361 | 0.0092424 | 4.5639377 |
| H | 14.7699037 | -0.7756969 | 3.7940407 |

**5(AuCl)a**

Energy = -1404.121657265

| | | | |
|---|---|---|---|
| C | -0.1526201 | -0.5069612 | -0.5920929 |
| C | -1.6431120 | -0.5083402 | -0.7275494 |
| C | -2.6262118 | -0.9958218 | 0.1427099 |
| H | -2.3426037 | -1.4975361 | 1.0786573 |
| C | -3.9773661 | -0.8398346 | -0.2162065 |
| H | -4.7649815 | -1.2178541 | 0.4501660 |
| C | -4.3295011 | -0.2085204 | -1.4250120 |
| H | -5.3906332 | -0.0999965 | -1.6898222 |
| C | -3.3428576 | 0.2855548 | -2.2988452 |
| H | -3.6310940 | 0.7823446 | -3.2358600 |
| C | -1.9927272 | 0.1350416 | -1.9486845 |
| C | -0.7542367 | 0.5591569 | -2.6267819 |
| C | -0.5421491 | 1.2453712 | -3.8318795 |
| H | -1.3877454 | 1.5521802 | -4.4633441 |
| C | 0.7778409 | 1.5411506 | -4.2209375 |
| H | 0.9572647 | 2.0752669 | -5.1645637 |

| | | | |
|---|---|---|---|
| C | 1.8722664 | 1.1630056 | -3.4190307 |
| H | 2.8939388 | 1.4045023 | -3.7432952 |
| C | 1.6691377 | 0.4741053 | -2.2095130 |
| H | 2.5181830 | 0.1652979 | -1.5834946 |
| C | 0.3565507 | 0.1758576 | -1.8226987 |
| C | 0.5820411 | -0.8169119 | 0.5547129 |
| C | 1.1021156 | -0.4147178 | 1.7519029 |
| C | 0.8466393 | 0.9766107 | 2.1535783 |
| H | 0.2509076 | 1.5465955 | 1.4240437 |
| C | 1.2297407 | 1.6598138 | 3.2764611 |
| H | 0.8960379 | 2.7081693 | 3.3218753 |
| C | 2.0066033 | 1.2223485 | 4.4180071 |
| H | 2.1717827 | 1.9852814 | 5.1939402 |
| C | 2.5516359 | -0.0148236 | 4.6391655 |
| H | 3.1129929 | -0.1510353 | 5.5760307 |
| C | 2.4820355 | -1.1828500 | 3.7848419 |
| H | 3.0016927 | -2.0703427 | 4.1776440 |
| C | 1.8739864 | -1.3552918 | 2.5708070 |
| H | 1.9687534 | -2.3556352 | 2.1201229 |
| Cl | 1.1155184 | -4.8023639 | -0.9532981 |
| Au | 0.6402239 | -2.6188579 | -0.4617371 |

**5(AuCl)b**

Energy = -1404.118834225

| | | | |
|---|---|---|---|
| C | 0.0162140 | 0.5207410 | -1.3669864 |
| C | -0.7126940 | -0.0980158 | -0.2244461 |
| C | -2.0460930 | -0.4833759 | -0.7498273 |
| C | -2.1157646 | -0.1183732 | -2.1266408 |
| C | -0.8364401 | 0.5037347 | -2.5097615 |
| C | -3.2806811 | -0.3733230 | -2.8665654 |
| C | -4.3693802 | -0.9916808 | -2.2251748 |
| C | -4.2975390 | -1.3508911 | -0.8649183 |
| C | -3.1338260 | -1.0991471 | -0.1159751 |
| C | 1.3075505 | 1.0599982 | -1.4424266 |
| C | 1.7501484 | 1.5863123 | -2.6701333 |
| C | 0.9109808 | 1.5711437 | -3.8012301 |
| C | -0.3861019 | 1.0309673 | -3.7301310 |
| C | -0.2229739 | -0.2565005 | 1.0150585 |
| Au | -0.8729512 | -1.0651280 | 2.9067147 |
| Cl | -1.9814950 | -2.0316727 | 4.6645547 |
| C | 0.8088142 | -0.1120570 | 1.9816095 |
| C | 1.9192349 | -1.0939153 | 1.9744584 |
| C | 2.9432494 | -1.2436550 | 2.8717995 |
| C | 3.2597464 | -0.4665138 | 4.0457932 |
| C | 2.7591581 | 0.7639094 | 4.3946730 |
| C | 1.8018113 | 1.5617768 | 3.6672403 |
| C | 0.9815551 | 1.2106002 | 2.6280327 |
| H | -3.0774169 | -1.3790982 | 0.9459727 |
| H | -5.1591825 | -1.8328486 | -0.3825373 |
| H | -5.2882159 | -1.1972773 | -2.7923152 |
| H | -3.3465068 | -0.0967135 | -3.9283322 |
| H | -1.0327076 | 1.0240296 | -4.6189417 |

| | | | |
|---|---|---|---|
| H | 1.2747534 | 1.9867351 | -4.7515101 |
| H | 2.7599982 | 2.0129651 | -2.7472168 |
| H | 1.9651226 | 1.0734256 | -0.5617823 |
| H | 0.3172460 | 1.9927512 | 2.2295849 |
| H | 1.7099699 | 2.6048922 | 4.0080484 |
| H | 3.1707661 | 1.2299144 | 5.3026060 |
| H | 4.0343916 | -0.8929783 | 4.7008026 |
| H | 3.6201043 | -2.0901651 | 2.6771324 |
| H | 1.8684293 | -1.8197348 | 1.1484179 |

**5$(AuCl)_2$a**

Energy = -2000.1862038870

| | | | |
|---|---|---|---|
| C | -2.536037 | -0.824126 | -3.376278 |
| C | -1.742934 | -0.301173 | -2.348730 |
| C | -1.966762 | -0.675265 | -0.986471 |
| C | -3.005936 | -1.569257 | -0.670992 |
| C | -3.803639 | -2.085873 | -1.706676 |
| C | -3.572318 | -1.719618 | -3.045482 |
| C | -0.619478 | 0.647668 | -2.389329 |
| C | -0.147267 | 0.831716 | -1.052869 |
| C | -0.934106 | -0.031804 | -0.143530 |
| C | -0.040280 | 1.351207 | -3.451832 |
| C | 1.001447 | 2.260170 | -3.179150 |
| C | 1.441498 | 2.477070 | -1.859640 |
| C | 0.862584 | 1.774534 | -0.787929 |
| C | -0.712226 | -0.178410 | 1.250552 |
| Au | -1.591367 | -1.711117 | 2.403169 |
| Cl | -2.257728 | -3.654527 | 3.446103 |
| C | 0.615644 | -0.030857 | 1.846385 |
| C | 1.715271 | -0.672273 | 1.168435 |
| C | 3.046178 | -0.803558 | 1.533746 |
| C | 3.728850 | -0.334235 | 2.695274 |
| C | 3.205869 | 0.401611 | 3.745835 |
| C | 1.859663 | 0.842296 | 3.917234 |
| C | 0.747829 | 0.637862 | 3.114699 |
| Au | -2.360999 | 0.956639 | 2.010839 |
| Cl | -3.784215 | 2.586688 | 2.792832 |
| H | 1.180750 | 1.988308 | 0.240492 |
| H | 2.230610 | 3.215784 | -1.663076 |
| H | 1.460165 | 2.823530 | -4.003781 |
| H | -0.397934 | 1.212891 | -4.481608 |
| H | -2.358179 | -0.544732 | -4.424129 |
| H | -4.207868 | -2.133320 | -3.840875 |
| H | -4.619968 | -2.778951 | -1.462414 |
| H | -3.202008 | -1.856837 | 0.372269 |
| H | -0.197556 | 1.064501 | 3.488239 |
| H | 1.671340 | 1.424701 | 4.831691 |
| H | 3.904565 | 0.679901 | 4.548946 |
| H | 4.797957 | -0.587445 | 2.754085 |
| H | 3.671710 | -1.360033 | 0.819374 |
| H | 1.438315 | -1.158019 | 0.221335 |

**5$(AuCl)_2$b**

Energy = -2000.192224984

| | | | |
|---|---|---|---|
| C | -0.5254573 | -0.5961237 | -0.3965707 |
| C | -1.8985802 | -0.6974595 | -0.9782735 |
| C | -3.0243361 | -1.4271067 | -0.5662288 |
| H | -2.9723285 | -2.0941582 | 0.3066953 |
| C | -4.2212000 | -1.2985610 | -1.2928266 |
| H | -5.1054936 | -1.8697985 | -0.9792320 |
| C | -4.2946538 | -0.4536884 | -2.4162597 |
| H | -5.2389524 | -0.3688880 | -2.9720770 |
| C | -3.1713473 | 0.2815127 | -2.8363154 |
| H | -3.2365783 | 0.9427348 | -3.7117021 |
| C | -1.9733642 | 0.1556701 | -2.1184231 |
| C | -0.6614865 | 0.7906581 | -2.3192833 |
| C | -0.2098151 | 1.6894534 | -3.2970003 |
| H | -0.8854880 | 2.0491841 | -4.0854592 |
| C | 1.1290184 | 2.1200597 | -3.2596507 |
| H | 1.4963325 | 2.8196337 | -4.0235315 |
| C | 2.0089442 | 1.6518560 | -2.2655145 |
| H | 3.0568047 | 1.9823297 | -2.2650990 |
| C | 1.5631239 | 0.7495685 | -1.2825905 |
| H | 2.2671121 | 0.3613767 | -0.5344068 |
| C | 0.2229529 | 0.3328495 | -1.3002709 |
| C | -0.0889856 | -1.0296152 | 0.8878754 |
| C | 0.9210285 | -0.3837626 | 1.7097140 |
| C | 0.7331504 | 1.0252377 | 1.9740781 |
| H | -0.1373502 | 1.4654769 | 1.4654754 |
| C | 1.4623766 | 1.8889221 | 2.7712452 |
| H | 1.0944607 | 2.9261725 | 2.7915009 |
| C | 2.6196956 | 1.6439504 | 3.5724499 |
| H | 3.0016438 | 2.5096249 | 4.1337195 |
| C | 3.3150928 | 0.4559521 | 3.7136010 |
| H | 4.1959100 | 0.4765756 | 4.3727733 |
| C | 3.0332564 | -0.8032945 | 3.1018783 |
| H | 3.7414831 | -1.6094515 | 3.3454991 |
| C | 1.9998332 | -1.1680968 | 2.2555238 |
| H | 1.9935645 | -2.2199816 | 1.9292279 |
| Cl | 1.2785261 | -4.6481498 | -1.1486971 |
| Cl | -2.6693446 | -3.0250077 | 3.7777811 |
| Au | -1.2432843 | -1.9517913 | 2.3142611 |
| Au | 0.4237145 | -2.6738532 | -0.3738968 |

**5$(AuCl)_2$c**

Energy = -2000.193296876

| | | | |
|---|---|---|---|
| C | -0.4940650 | -0.5901626 | -0.4550033 |
| C | -1.8782031 | -0.6966695 | -1.0088529 |
| C | -2.9934020 | -1.4200271 | -0.5608032 |
| H | -2.9233071 | -2.0688084 | 0.3241877 |
| C | -4.2033933 | -1.3051561 | -1.2678816 |
| H | -5.0825543 | -1.8693362 | -0.9281202 |
| C | -4.2969361 | -0.4805201 | -2.4050399 |
| H | -5.2514377 | -0.4058121 | -2.9446303 |

| | | | |
|---|---|---|---|
| C | -3.1830336 | 0.2492434 | -2.8585901 |
| H | -3.2661909 | 0.8958533 | -3.7433164 |
| C | -1.9720291 | 0.1385774 | -2.1598873 |
| C | -0.6656594 | 0.7787109 | -2.3857006 |
| C | -0.2317825 | 1.6739981 | -3.3747214 |
| H | -0.9173024 | 2.0195182 | -4.1610241 |
| C | 1.1015223 | 2.1226674 | -3.3489785 |
| H | 1.4543455 | 2.8206060 | -4.1211407 |
| C | 1.9932696 | 1.6797963 | -2.3535607 |
| H | 3.0348348 | 2.0294532 | -2.3598998 |
| C | 1.5662844 | 0.7808014 | -1.3592264 |
| H | 2.2753197 | 0.4157465 | -0.6037969 |
| C | 0.2343389 | 0.3410160 | -1.3717848 |
| C | -0.0412589 | -1.0083768 | 0.8237163 |
| C | 0.9260042 | -0.3987956 | 1.7140858 |
| C | 0.7395567 | 1.0107377 | 2.0074948 |
| H | -0.1012219 | 1.4726912 | 1.4685655 |
| C | 1.4349510 | 1.8408898 | 2.8625187 |
| H | 1.0750624 | 2.8805942 | 2.8966435 |
| C | 2.5488883 | 1.5593607 | 3.7173650 |
| H | 2.8924102 | 2.3981047 | 4.3409419 |
| C | 3.2482828 | 0.3739167 | 3.8306583 |
| H | 4.0948466 | 0.3654430 | 4.5334677 |
| C | 3.0202988 | -0.8512514 | 3.1258736 |
| H | 3.7449058 | -1.6519075 | 3.3378759 |
| C | 2.0262422 | -1.1873505 | 2.2283476 |
| H | 2.0616743 | -2.2131358 | 1.8289862 |
| Cl | 1.2531851 | -4.6393476 | -1.2112922 |
| Cl | -2.5331246 | -2.6651606 | 3.9859725 |
| Au | -1.1319703 | -1.7518734 | 2.4053054 |
| Au | 0.4406284 | -2.6440244 | -0.4487654 |

**5($H^+$)**

Energy = -808.4625258258

| | | | |
|---|---|---|---|
| C | -0.5511312 | -0.3086764 | -0.3069637 |
| C | -1.8654277 | -0.6754683 | -0.8672185 |
| C | -2.8856801 | -1.4892968 | -0.3435888 |
| H | -2.7631504 | -2.0230460 | 0.6092782 |
| C | -4.0852780 | -1.6218362 | -1.0659981 |
| H | -4.8889732 | -2.2601752 | -0.6761604 |
| C | -4.2625054 | -0.9415227 | -2.2842365 |
| H | -5.2072995 | -1.0537331 | -2.8333883 |
| C | -3.2457991 | -0.1149036 | -2.8141000 |
| H | -3.4045626 | 0.4145768 | -3.7630974 |
| C | -2.0493268 | 0.0089166 | -2.1053717 |
| C | -0.8116999 | 0.7583595 | -2.3958763 |
| C | -0.4428764 | 1.5086186 | -3.5146688 |
| H | -1.1451131 | 1.6719102 | -4.3431292 |
| C | 0.8647643 | 2.0359335 | -3.5793765 |
| H | 1.1681810 | 2.6265304 | -4.4545611 |
| C | 1.7924414 | 1.7887192 | -2.5523696 |
| H | 2.8171659 | 2.1736027 | -2.6386442 |

| | | | |
|---|---|---|---|
| C | 1.4218382 | 1.0411776 | -1.4200431 |
| H | 2.1755918 | 0.8274484 | -0.6514193 |
| C | 0.1055252 | 0.5515087 | -1.3157143 |
| C | -0.1235509 | -0.7865323 | 0.9310530 |
| C | 0.9159523 | -0.3495853 | 1.8233393 |
| C | 1.3920836 | 1.0061762 | 1.7856116 |
| H | 0.8715844 | 1.6547510 | 1.0674764 |
| C | 2.3720106 | 1.6379968 | 2.5413599 |
| H | 2.5233385 | 2.7030560 | 2.3087638 |
| C | 3.2104124 | 1.1230976 | 3.5693670 |
| H | 3.9453330 | 1.8285955 | 3.9845420 |
| C | 3.1869089 | -0.1495224 | 4.1259039 |
| H | 3.9108687 | -0.3504457 | 4.9292607 |
| C | 2.3103961 | -1.2214110 | 3.7993477 |
| H | 2.4381230 | -2.1300421 | 4.4067975 |
| C | 1.3261166 | -1.3002583 | 2.8222091 |
| H | 0.7889656 | -2.2605870 | 2.7842063 |
| H | -0.7026674 | -1.6420043 | 1.3128596 |

**5($H^+$)$_2$**

Energy = -808.6948044053

| | | | |
|---|---|---|---|
| C | -0.3778510 | -0.7179075 | -0.5252631 |
| C | -1.7885191 | -0.6475574 | -0.7840333 |
| C | -2.8840061 | -1.2157352 | -0.0854304 |
| H | -2.7374783 | -1.8266549 | 0.8166483 |
| C | -4.1822491 | -0.9939076 | -0.5754029 |
| H | -5.0484043 | -1.4255540 | -0.0577189 |
| C | -4.3738654 | -0.2236906 | -1.7365964 |
| H | -5.3947549 | -0.0616847 | -2.1105618 |
| C | -3.2782911 | 0.3529439 | -2.4523172 |
| H | -3.4720086 | 0.9435581 | -3.3575950 |
| C | -1.9964275 | 0.1378453 | -1.9756841 |
| C | -0.6568675 | 0.5542678 | -2.4657807 |
| C | -0.2496396 | 1.2830388 | -3.5713776 |
| H | -0.9679756 | 1.7017792 | -4.2887173 |
| C | 1.1507276 | 1.4776205 | -3.7778906 |
| H | 1.4832932 | 2.0513629 | -4.6543800 |
| C | 2.1108524 | 0.9478058 | -2.8980394 |
| H | 3.1784800 | 1.1079706 | -3.0958339 |
| C | 1.7031531 | 0.2061686 | -1.7749232 |
| H | 2.4562484 | -0.2195945 | -1.0970201 |
| C | 0.3182954 | 0.0131905 | -1.5546542 |
| C | 0.2674349 | -1.4879988 | 0.5930917 |
| C | 1.0064692 | -0.7006196 | 1.6796204 |
| C | 0.5710489 | 0.6110276 | 1.9858911 |
| H | -0.2528900 | 0.9982916 | 1.3663347 |
| C | 1.0239548 | 1.5041098 | 2.9721666 |
| H | 0.5030739 | 2.4737194 | 2.9988686 |
| C | 2.0403955 | 1.3400704 | 3.9347472 |
| H | 2.2082528 | 2.1951818 | 4.6072563 |
| C | 2.8581189 | 0.2175133 | 4.1410389 |
| H | 3.5939767 | 0.2936387 | 4.9562004 |

| | | | |
|---|---|---|---|
| C | 2.8480396 | -1.0002451 | 3.4310161 |
| H | 3.5796224 | -1.7506537 | 3.7686058 |
| C | 2.0406649 | -1.3991157 | 2.3528556 |
| H | 2.2445679 | -2.4169576 | 1.9839481 |
| H | 0.9709355 | -2.2174829 | 0.1398283 |
| H | -0.4963677 | -2.1057451 | 1.1111117 |

**6**

Energy = -1115.154370734

| | | | |
|---|---|---|---|
| C | 1.2748665 | 6.5295527 | 3.0040961 |
| C | 1.8383834 | 5.7541661 | 3.9275845 |
| C | 2.3662058 | 4.9911857 | 4.8832831 |
| C | 1.7077861 | 4.5681364 | 6.1486801 |
| C | 0.4269580 | 4.8469071 | 6.6432482 |
| H | -0.2692354 | 5.4715876 | 6.0659666 |
| C | 0.0549207 | 4.3114309 | 7.8893840 |
| H | -0.9458295 | 4.5186753 | 8.2939947 |
| C | 0.9517341 | 3.5111924 | 8.6256903 |
| H | 0.6410826 | 3.1027830 | 9.5977794 |
| C | 2.2380332 | 3.2291174 | 8.1324525 |
| H | 2.9302051 | 2.6039236 | 8.7142725 |
| C | 2.6190908 | 3.7592185 | 6.8888324 |
| C | 3.8703779 | 3.6462876 | 6.1212869 |
| C | 5.0726110 | 2.9732868 | 6.3944615 |
| H | 5.1977122 | 2.4000458 | 7.3240700 |
| C | 6.1200544 | 3.0428305 | 5.4586096 |
| H | 7.0655805 | 2.5203001 | 5.6615286 |
| C | 5.9727732 | 3.7745094 | 4.2632296 |
| H | 6.8035807 | 3.8157422 | 3.5448338 |
| C | 4.7726409 | 4.4519646 | 3.9810232 |
| H | 4.6575895 | 5.0228796 | 3.0482661 |
| C | 3.7255429 | 4.3860165 | 4.9104106 |
| C | 0.5393198 | 5.8922473 | 1.8649089 |
| C | 1.1329305 | 4.7862285 | 1.2178910 |
| H | 2.1394112 | 4.4764209 | 1.5304306 |
| C | 0.4641549 | 4.0807148 | 0.2089551 |
| H | 0.9510211 | 3.2222920 | -0.2742883 |
| C | -0.8323313 | 4.4707590 | -0.1672578 |
| H | -1.3738050 | 3.9213420 | -0.9500145 |
| C | -1.4329105 | 5.5646444 | 0.4627965 |
| H | -2.4480071 | 5.8720050 | 0.1714371 |
| C | -0.7664948 | 6.3115634 | 1.4696564 |
| C | -1.4792776 | 7.4511375 | 2.0437090 |
| H | -2.5652133 | 7.4436342 | 1.8577986 |
| C | -0.9913918 | 8.5574902 | 2.6760175 |
| H | -1.7336442 | 9.3291997 | 2.9354847 |
| C | 0.3900866 | 8.9345768 | 2.9685068 |
| C | 0.6605275 | 10.3128921 | 3.1755477 |
| H | -0.1768547 | 11.0234890 | 3.1147872 |
| C | 1.9505530 | 10.7828672 | 3.4384112 |
| H | 2.1254054 | 11.8581025 | 3.5836263 |
| C | 3.0172131 | 9.8714703 | 3.5167050 |

| | | | |
|---|---|---|---|
| H | 4.0374266 | 10.2229120 | 3.7243921 |
| C | 2.7718462 | 8.5032857 | 3.3414020 |
| H | 3.5972496 | 7.7826942 | 3.4197759 |
| C | 1.4743845 | 8.0127543 | 3.0765449 |

**6(AuCl)a**

Energy = -1711.219745707

| | | | |
|---|---|---|---|
| C | -0.2380481 | 1.1095799 | -0.7663281 |
| C | 0.4055788 | 0.6371529 | 0.3197827 |
| C | 0.7929480 | -0.4386085 | 1.1265465 |
| C | -0.0774137 | -1.1573048 | 2.1053052 |
| C | -1.3434835 | -0.8227294 | 2.6015066 |
| H | -1.8326978 | 0.1132598 | 2.2977889 |
| C | -1.9643763 | -1.7065118 | 3.5023773 |
| H | -2.9561979 | -1.4625994 | 3.9073378 |
| C | -1.3248245 | -2.8988582 | 3.8935658 |
| H | -1.8254143 | -3.5743471 | 4.6013815 |
| C | -0.0553993 | -3.2391504 | 3.3904349 |
| H | 0.4290815 | -4.1769540 | 3.6963568 |
| C | 0.5719993 | -2.3637868 | 2.4915498 |
| C | 1.8634106 | -2.4480934 | 1.7865010 |
| C | 2.8675318 | -3.4280253 | 1.8013795 |
| H | 2.7685833 | -4.3264095 | 2.4265862 |
| C | 4.0084372 | -3.2447941 | 0.9983640 |
| H | 4.8031820 | -4.0038269 | 1.0048066 |
| C | 4.1484071 | -2.1007024 | 0.1890746 |
| H | 5.0499176 | -1.9751957 | -0.4262850 |
| C | 3.1477855 | -1.1120984 | 0.1690438 |
| H | 3.2627969 | -0.2080952 | -0.4456272 |
| C | 2.0093458 | -1.2937520 | 0.9653632 |
| C | -0.8717775 | 0.1283626 | -1.7021066 |
| C | -0.1132642 | -0.9699660 | -2.1625722 |
| H | 0.9435248 | -1.0405376 | -1.8729558 |
| C | -0.6829825 | -1.9653703 | -2.9670443 |
| H | -0.0689977 | -2.8096178 | -3.3099903 |
| C | -2.0418163 | -1.8830284 | -3.3162058 |
| H | -2.5049839 | -2.6636281 | -3.9357614 |
| C | -2.8048361 | -0.8003634 | -2.8699652 |
| H | -3.8682279 | -0.7327263 | -3.1426457 |
| C | -2.2444202 | 0.2379920 | -2.0807398 |
| C | -3.1193412 | 1.3440841 | -1.6969509 |
| H | -4.1952922 | 1.1201631 | -1.7729223 |
| C | -2.7952086 | 2.6300845 | -1.3742804 |
| H | -3.6414259 | 3.3185877 | -1.2209737 |
| C | -1.4807953 | 3.2666983 | -1.3207887 |
| C | -1.4229860 | 4.6735306 | -1.4980925 |
| H | -2.3648973 | 5.2208970 | -1.6487805 |
| C | -0.2091359 | 5.3670732 | -1.5009259 |
| H | -0.1985814 | 6.4557415 | -1.6499658 |
| C | 0.9927221 | 4.6648534 | -1.3105746 |
| H | 1.9548626 | 5.1948975 | -1.3078998 |
| C | 0.9590403 | 3.2799257 | -1.1003676 |

| | | | |
|---|---|---|---|
| H | 1.8947736 | 2.7283453 | -0.9366168 |
| C | -0.2595289 | 2.5659621 | -1.0876759 |
| Cl | 2.2546534 | 3.2020144 | 3.2576034 |
| Au | 1.3780021 | 1.5879957 | 1.8924372 |

**6(AuCl)b**

Energy = -1711.223010483

| | | | |
|---|---|---|---|
| C | -0.3175449 | 2.1753565 | -0.8673959 |
| C | -0.9659433 | 3.2412167 | -1.5661487 |
| C | -0.3575202 | 4.5246075 | -1.5473054 |
| C | 0.8625179 | 4.7562458 | -0.9097732 |
| C | 1.5048078 | 3.6998879 | -0.2395813 |
| C | 0.9080114 | 2.4356319 | -0.2083175 |
| C | -2.2330613 | 3.1243218 | -2.2754121 |
| C | -2.8182233 | 2.0223817 | -2.8273618 |
| C | -2.3445804 | 0.6453280 | -2.8665983 |
| C | -1.4380344 | 0.0642396 | -1.9257413 |
| C | -1.0724971 | -1.2949293 | -2.0780004 |
| C | -1.5615364 | -2.0733385 | -3.1317101 |
| C | -2.4678594 | -1.5123607 | -4.0490201 |
| C | -2.8568983 | -0.1797454 | -3.9030806 |
| C | -0.9076371 | 0.8021669 | -0.7313911 |
| C | -0.6746296 | 0.0821459 | 0.4588608 |
| Au | -2.5476318 | 0.8754036 | 0.8421136 |
| Cl | -4.5446185 | 1.4250724 | 1.8247372 |
| C | 0.1334198 | -0.7127908 | 1.1944795 |
| C | -0.0960206 | -1.2684099 | 2.5517638 |
| C | 1.0373977 | -2.0528929 | 2.9206702 |
| C | 2.0092491 | -2.0171976 | 1.8167340 |
| C | 1.4730291 | -1.2101326 | 0.7690491 |
| C | 1.0816584 | -2.6974805 | 4.1663734 |
| C | -0.0090761 | -2.5561562 | 5.0426190 |
| C | -1.1278087 | -1.7816510 | 4.6788192 |
| C | -1.1797445 | -1.1327475 | 3.4323008 |
| C | 2.2001923 | -1.0055095 | -0.4141838 |
| C | 3.4647068 | -1.6087826 | -0.5486789 |
| C | 3.9941038 | -2.4050108 | 0.4848521 |
| C | 3.2711722 | -2.6144985 | 1.6731533 |
| H | -2.0575680 | -0.5302652 | 3.1572835 |
| H | -1.9717504 | -1.6812474 | 5.3752561 |
| H | 0.0111718 | -3.0551306 | 6.0217680 |
| H | 1.9517715 | -3.3033337 | 4.4562857 |
| H | 3.6920896 | -3.2374524 | 2.4750132 |
| H | 4.9833192 | -2.8678462 | 0.3613678 |
| H | 4.0432589 | -1.4559582 | -1.4703824 |
| H | 1.7979344 | -0.3863567 | -1.2279552 |
| H | -0.3947284 | -1.7469422 | -1.3431420 |
| H | -1.2497799 | -3.1225719 | -3.2249920 |
| H | -2.8762307 | -2.1182748 | -4.8697337 |
| H | -3.5746642 | 0.2597770 | -4.6104553 |
| H | -3.7398243 | 2.2017915 | -3.4024690 |
| H | -2.7401944 | 4.0840910 | -2.4598178 |

| | | | |
|---|---|---|---|
| H | -0.8693624 | 5.3500280 | -2.0625284 |
| H | 1.3099277 | 5.7597569 | -0.9253181 |
| H | 2.4612578 | 3.8642302 | 0.2751744 |
| H | 1.3940790 | 1.6235626 | 0.3465796 |

**6$(AuCl)_2$a**

Energy = -2307.267072633

| | | | |
|---|---|---|---|
| C | 3.4233246 | -2.3261813 | 1.8099897 |
| C | 2.1549707 | -1.7425089 | 1.9231040 |
| C | 1.4814748 | -1.2478457 | 0.7678387 |
| C | 2.0794869 | -1.3517179 | -0.4990015 |
| C | 3.3541166 | -1.9356019 | -0.6063183 |
| C | 4.0183602 | -2.4187890 | 0.5370842 |
| C | 0.1640471 | -0.6915330 | 1.1825517 |
| C | 0.0764062 | -0.9076268 | 2.6473250 |
| C | 1.2898394 | -1.5180002 | 3.0915951 |
| C | 1.4993864 | -1.7910153 | 4.4479872 |
| C | 0.4897560 | -1.4565265 | 5.3717190 |
| C | -0.7057233 | -0.8528462 | 4.9409113 |
| C | -0.9206742 | -0.5734541 | 3.5800435 |
| C | -0.7952639 | -0.1457141 | 0.2912634 |
| Au | -2.5760316 | 0.7434858 | 0.9704160 |
| Cl | -4.4390010 | 1.5147921 | 2.0762442 |
| C | 1.3792875 | 2.0341963 | -0.0359539 |
| C | 0.0774630 | 2.0666508 | -0.5935787 |
| C | -0.5075086 | 3.3449855 | -0.8841279 |
| C | 0.2378429 | 4.5152712 | -0.5760888 |
| C | 1.5300395 | 4.4563107 | -0.0566204 |
| C | 2.1075748 | 3.2014216 | 0.2082407 |
| C | -0.6831356 | 0.7960395 | -0.7820443 |
| Au | -1.8354056 | -1.9673988 | 0.0578939 |
| Cl | -3.1415241 | -3.7560844 | -0.5598877 |
| C | -1.8449982 | 3.5522988 | -1.4194117 |
| C | -2.5867703 | 2.7301973 | -2.2184944 |
| C | -2.2264962 | 1.4237323 | -2.7425302 |
| C | -1.3230403 | 0.5224845 | -2.0947799 |
| C | -1.0549740 | -0.7279201 | -2.7095811 |
| C | -1.6453649 | -1.0928907 | -3.9233859 |
| C | -2.5643751 | -0.2244361 | -4.5383108 |
| C | -2.8552698 | 1.0046277 | -3.9443701 |
| H | -1.8623200 | -0.1058485 | 3.2570786 |
| H | -1.4851094 | -0.5979734 | 5.6715537 |
| H | 0.6383930 | -1.6685463 | 6.4397703 |
| H | 2.4340487 | -2.2555783 | 4.7916733 |
| H | 3.9474227 | -2.7105461 | 2.6959523 |
| H | 5.0113251 | -2.8781930 | 0.4339872 |
| H | 3.8312990 | -2.0211061 | -1.5920247 |
| H | 1.5687949 | -0.9826394 | -1.3983465 |
| H | -0.3594958 | -1.4250425 | -2.2243204 |
| H | -1.4100403 | -2.0674720 | -4.3711659 |
| H | -3.0584814 | -0.5133274 | -5.4761409 |
| H | -3.5819772 | 1.6815721 | -4.4154519 |

| | | | |
|---|---|---|---|
| H | -3.5369342 | 3.1380627 | -2.5959066 |
| H | -2.2656042 | 4.5506751 | -1.2243488 |
| H | -0.2290237 | 5.4914469 | -0.7698640 |
| H | 2.0843611 | 5.3815105 | 0.1529793 |
| H | 3.1223323 | 3.1302153 | 0.6230730 |
| H | 1.8394014 | 1.0704742 | 0.2003541 |

**6$(AuCl)_2$b**

Energy = -2307.260664923

| | | | |
|---|---|---|---|
| C | 0.2983483 | -0.4571084 | 1.3652170 |
| C | -0.0554650 | -1.3966709 | 2.4781091 |
| C | 1.0181499 | -2.3211709 | 2.6526267 |
| C | 2.0766200 | -2.0094612 | 1.6842652 |
| C | 1.6525688 | -0.9058823 | 0.8905178 |
| C | 2.4780117 | -0.4219026 | -0.1376569 |
| H | 2.1664729 | 0.4190974 | -0.7703085 |
| C | 3.7214595 | -1.0368689 | -0.3662110 |
| H | 4.3709535 | -0.6636921 | -1.1698442 |
| C | 4.1426231 | -2.1196087 | 0.4285622 |
| H | 5.1218180 | -2.5824189 | 0.2422963 |
| C | 3.3216363 | -2.6147482 | 1.4568905 |
| H | 3.6524247 | -3.4644917 | 2.0701613 |
| C | 0.9425138 | -3.3404581 | 3.6118399 |
| H | 1.7703911 | -4.0516260 | 3.7407817 |
| C | -0.2142904 | -3.4443758 | 4.4042604 |
| H | -0.2867981 | -4.2361446 | 5.1629523 |
| C | -1.2800027 | -2.5424851 | 4.2308446 |
| H | -2.1803725 | -2.6308029 | 4.8537677 |
| C | -1.2083266 | -1.5169037 | 3.2723481 |
| H | -2.0474237 | -0.8134473 | 3.1617857 |
| C | -0.4966193 | 0.5556538 | 0.7288047 |
| Au | 0.5361454 | 1.6187471 | 2.3293345 |
| Cl | 1.4095199 | 3.1631156 | 3.7779105 |
| Au | -2.2711513 | 1.1173945 | 1.6576330 |
| Cl | -4.2546439 | 1.5009212 | 2.7811704 |
| C | -0.4869910 | 0.9475659 | -0.6571906 |
| C | -0.9587735 | -0.0465907 | -1.6523470 |
| C | -0.5174073 | -1.3941420 | -1.5352895 |
| H | 0.1921435 | -1.6575918 | -0.7470171 |
| C | -0.9259721 | -2.3954026 | -2.4143877 |
| H | -0.5291478 | -3.4128095 | -2.2967085 |
| C | -1.8578684 | -2.1022919 | -3.4283016 |
| H | -2.2043781 | -2.8868138 | -4.1148983 |
| C | -2.3547275 | -0.8068039 | -3.5337131 |
| H | -3.1074699 | -0.5727233 | -4.2995870 |
| C | -1.9212251 | 0.2498007 | -2.6837624 |
| C | -2.5826853 | 1.5229369 | -2.8929226 |
| H | -3.4997720 | 1.4595222 | -3.4982132 |
| C | -2.1970891 | 2.7795900 | -2.5246458 |
| H | -2.8408790 | 3.6051977 | -2.8639304 |
| C | -0.9847172 | 3.1927801 | -1.8507747 |
| C | -0.1706807 | 2.3456589 | -1.0212159 |

| | | | |
|---|---|---|---|
| C | 1.0032342 | 2.9149450 | -0.4509450 |
| H | 1.6634085 | 2.2805466 | 0.1537263 |
| C | 1.3692636 | 4.2461894 | -0.6594289 |
| H | 2.2908175 | 4.6313744 | -0.2036855 |
| C | 0.5384945 | 5.0833105 | -1.4249215 |
| H | 0.7962973 | 6.1410494 | -1.5722543 |
| H | -1.2750250 | 5.2065008 | -2.5950292 |
| C | -0.6191287 | 4.5580541 | -1.9974252 |

**6$(AuCl)_2$b'**

Energy = -2307.261305476

| | | | |
|---|---|---|---|
| C | -0.3319008 | 2.3071853 | -1.0245959 |
| C | -1.0479613 | 3.1909438 | -1.8930150 |
| C | -0.6184859 | 4.5428996 | -1.9921539 |
| C | 0.5207087 | 5.0035935 | -1.3351542 |
| C | 1.2639171 | 4.1186751 | -0.5301682 |
| C | 0.8237385 | 2.8056567 | -0.3595147 |
| C | -2.2006996 | 2.8110269 | -2.6819090 |
| C | -2.5368841 | 1.5670981 | -3.1334150 |
| C | -1.8852985 | 0.2879981 | -2.9139831 |
| C | -1.0520932 | -0.0622811 | -1.7895977 |
| C | -0.6221263 | -1.4127634 | -1.6843573 |
| C | -0.9054529 | -2.3653667 | -2.6616416 |
| C | -1.6982237 | -2.0176700 | -3.7718771 |
| C | -2.1941458 | -0.7207499 | -3.8686445 |
| C | -0.7153656 | 0.9063935 | -0.7007962 |
| Au | -2.7201810 | 0.5862746 | 0.5066145 |
| Au | -1.0619200 | 2.1016241 | 2.0256626 |
| Cl | -0.8878627 | 3.8649029 | 3.4962497 |
| C | -0.5324207 | 0.4781153 | 0.6874022 |
| C | 0.2284452 | -0.5554409 | 1.2313496 |
| C | -0.0415406 | -1.3002512 | 2.4783156 |
| C | 1.0489725 | -2.1868922 | 2.7322507 |
| C | 2.0575928 | -1.9851304 | 1.6808529 |
| C | 1.5649647 | -0.9981589 | 0.7699746 |
| C | 1.0248830 | -3.0492262 | 3.8361609 |
| C | -0.0921654 | -3.0225940 | 4.6925887 |
| C | -1.1681033 | -2.1474490 | 4.4467951 |
| C | -1.1513996 | -1.2813927 | 3.3403304 |
| C | 2.3538613 | -0.5888587 | -0.3204865 |
| C | 3.6183522 | -1.1739976 | -0.5074502 |
| C | 4.0952707 | -2.1527459 | 0.3855592 |
| C | 3.3189994 | -2.5633219 | 1.4858778 |
| Cl | -4.9828805 | 0.2315783 | 0.4027100 |
| H | -1.9902370 | -0.5936582 | 3.1626994 |
| H | -2.0291561 | -2.1368881 | 5.1287875 |
| H | -0.1243568 | -3.6906352 | 5.5646923 |
| H | 1.8591810 | -3.7365931 | 4.0346994 |
| H | 3.7034392 | -3.3215777 | 2.1823641 |
| H | 5.0877630 | -2.5966462 | 0.2249971 |
| H | 4.2405167 | -0.8612876 | -1.3572950 |
| H | 1.9960535 | 0.1728647 | -1.0260299 |

| | | | |
|---|---|---|---|
| H | -0.0421705 | -1.7218832 | -0.8116955 |
| H | -0.5259714 | -3.3894050 | -2.5444592 |
| H | -1.9480362 | -2.7647438 | -4.5376723 |
| H | -2.8494738 | -0.4497988 | -4.7082278 |
| H | -3.3905685 | 1.5210596 | -3.8264605 |
| H | -2.8118245 | 3.6484645 | -3.0514758 |
| H | -1.2012151 | 5.2278318 | -2.6240224 |
| H | 0.8350064 | 6.0505149 | -1.4454629 |
| H | 2.1678594 | 4.4619609 | -0.0099405 |
| H | 1.3881849 | 2.1336558 | 0.2997371 |

**6(AuCl)$_2$c**

Energy = -2307.280711940

| | | | |
|---|---|---|---|
| C | -0.6121366 | 0.9640079 | -0.6652004 |
| C | -0.2914003 | 0.4997199 | 0.6423263 |
| C | 0.4163978 | -0.4952718 | 1.3610628 |
| C | -0.1011216 | -1.4234611 | 2.4145844 |
| C | -1.3236721 | -1.4481451 | 3.1023935 |
| H | -2.0894138 | -0.6795533 | 2.9261203 |
| C | -1.5550421 | -2.4739101 | 4.0358374 |
| H | -2.5081440 | -2.4998673 | 4.5811825 |
| C | -0.5799291 | -3.4586985 | 4.2803638 |
| H | -0.7796665 | -4.2505370 | 5.0157661 |
| C | 0.6476949 | -3.4405864 | 3.5938923 |
| H | 1.4025753 | -4.2158619 | 3.7854251 |
| C | 0.8864670 | -2.4211079 | 2.6614608 |
| C | 2.0506451 | -2.1597951 | 1.8010774 |
| C | 3.2737945 | -2.8349106 | 1.6712552 |
| H | 3.4908255 | -3.7257381 | 2.2768605 |
| C | 4.2234052 | -2.3529159 | 0.7525840 |
| H | 5.1862620 | -2.8713678 | 0.6441758 |
| C | 3.9577024 | -1.2108656 | -0.0270098 |
| H | 4.7131643 | -0.8457267 | -0.7360652 |
| C | 2.7355169 | -0.5268117 | 0.0994774 |
| H | 2.5395389 | 0.3671095 | -0.5080866 |
| C | 1.7822415 | -1.0071790 | 1.0100001 |
| C | -0.9270190 | -0.0252273 | -1.7534354 |
| C | -0.1751615 | -1.2169523 | -1.8602664 |
| H | 0.6624707 | -1.3882607 | -1.1760770 |
| C | -0.4743834 | -2.1877359 | -2.8227363 |
| H | 0.1361628 | -3.0990602 | -2.8827599 |
| C | -1.5658977 | -2.0008048 | -3.6880880 |
| H | -1.8231024 | -2.7656086 | -4.4339372 |
| C | -2.3299061 | -0.8366661 | -3.5869082 |
| H | -3.1906222 | -0.6880692 | -4.2546469 |
| C | -2.0226307 | 0.1848424 | -2.6507443 |
| C | -2.8803903 | 1.3651690 | -2.6521025 |
| H | -3.8723886 | 1.2103262 | -3.1038451 |
| C | -2.5788122 | 2.6429300 | -2.2788641 |
| H | -3.3529318 | 3.4037577 | -2.4627641 |
| C | -1.3086677 | 3.1628173 | -1.7876751 |
| C | -1.0197098 | 4.5298253 | -2.0331047 |

| | | | |
|---|---|---|---|
| H | -1.7736264 | 5.1373639 | -2.5537381 |
| C | 0.1938706 | 5.1063774 | -1.6504532 |
| H | 0.3917473 | 6.1655525 | -1.8654284 |
| C | 1.1559379 | 4.3242152 | -0.9891810 |
| H | 2.1162240 | 4.7591330 | -0.6813841 |
| C | 0.8742002 | 2.9855738 | -0.6932482 |
| H | 1.6205355 | 2.3891263 | -0.1517800 |
| C | -0.3510322 | 2.3851809 | -1.0658821 |
| Cl | -4.4722181 | 1.2578153 | 1.5887052 |
| Cl | 1.2408332 | 3.1913547 | 3.7118331 |
| Au | 0.6003547 | 1.5587643 | 2.2481072 |
| Au | -2.3394917 | 0.9597228 | 0.8109309 |

**6($H^+$)**

Energy = -1115.543484300

| | | | |
|---|---|---|---|
| C | -0.8044157 | 0.9632225 | -0.5930226 |
| C | -0.6291630 | 0.3725125 | 0.7410698 |
| C | 0.1907594 | -0.6552932 | 1.1599235 |
| C | 0.1501042 | -1.2067628 | 2.5326824 |
| C | -0.6734552 | -0.8825518 | 3.6235877 |
| H | -1.4220688 | -0.0796710 | 3.5592328 |
| C | -0.5275981 | -1.6046091 | 4.8217189 |
| H | -1.1608889 | -1.3618421 | 5.6853230 |
| C | 0.4258584 | -2.6350215 | 4.9226625 |
| H | 0.5263517 | -3.1878116 | 5.8667222 |
| C | 1.2552582 | -2.9686559 | 3.8313585 |
| H | 1.9913292 | -3.7785782 | 3.9248283 |
| C | 1.1168107 | -2.2495122 | 2.6397119 |
| C | 1.8275194 | -2.3470031 | 1.3501971 |
| C | 2.8916832 | -3.1637280 | 0.9530918 |
| H | 3.3178587 | -3.9097904 | 1.6374419 |
| C | 3.4244249 | -3.0029147 | -0.3416949 |
| H | 4.2628869 | -3.6345698 | -0.6656815 |
| C | 2.9073028 | -2.0314859 | -1.2172973 |
| H | 3.3492004 | -1.9074860 | -2.2150707 |
| C | 1.8346343 | -1.2105486 | -0.8237841 |
| H | 1.4591402 | -0.4451941 | -1.5144332 |
| C | 1.2775052 | -1.3778501 | 0.4551669 |
| C | -1.2090418 | 0.0547187 | -1.6548446 |
| C | -1.5966375 | -1.2742865 | -1.2692756 |
| H | -1.7210473 | -1.4938564 | -0.2050208 |
| C | -1.8364865 | -2.2873255 | -2.1867763 |
| H | -2.1334598 | -3.2833824 | -1.8328931 |
| C | -1.7092508 | -2.0293660 | -3.5702989 |
| H | -1.8733005 | -2.8294985 | -4.3047491 |
| C | -1.4338970 | -0.7356184 | -3.9956977 |
| H | -1.4041884 | -0.5121694 | -5.0707133 |
| C | -1.2324216 | 0.3421096 | -3.0836878 |
| C | -1.1589106 | 1.6350674 | -3.6952173 |
| H | -1.2302787 | 1.6184204 | -4.7928608 |
| C | -1.1124008 | 2.8871912 | -3.1298954 |
| H | -1.1945083 | 3.7245648 | -3.8385976 |

| | | | |
|---|---|---|---|
| C | -0.9065771 | 3.2882405 | -1.7702609 |
| C | -0.8606428 | 4.7003215 | -1.5681000 |
| H | -1.0964097 | 5.3495322 | -2.4221356 |
| C | -0.4997370 | 5.2680100 | -0.3534068 |
| H | -0.4732273 | 6.3599727 | -0.2381953 |
| C | -0.1154767 | 4.4234749 | 0.7134217 |
| H | 0.2408173 | 4.8521604 | 1.6595502 |
| C | -0.1728848 | 3.0453916 | 0.5589997 |
| H | 0.1633277 | 2.4166089 | 1.3903670 |
| C | -0.6371089 | 2.4092315 | -0.6423799 |
| H | -1.2127045 | 0.8632530 | 1.5356442 |

**6($H^+$)$_2$**

Energy = -1115.788278936

| | | | |
|---|---|---|---|
| C | -0.9108208 | 0.8926909 | -0.6371197 |
| C | -0.9197897 | 0.3306341 | 0.7956433 |
| C | 0.1217360 | -0.6186245 | 1.3082092 |
| C | -0.0573579 | -1.3591631 | 2.5379848 |
| C | -1.1550988 | -1.4082150 | 3.4289599 |
| H | -2.0758844 | -0.8373293 | 3.2428934 |
| C | -1.0532721 | -2.2112830 | 4.5795417 |
| H | -1.8900815 | -2.2653952 | 5.2876573 |
| C | 0.1184915 | -2.9478519 | 4.8239835 |
| H | 0.1830329 | -3.5731149 | 5.7254665 |
| C | 1.2312745 | -2.9072777 | 3.9306417 |
| H | 2.1317024 | -3.4942594 | 4.1558108 |
| C | 1.1357917 | -2.1158476 | 2.7967421 |
| C | 2.0796406 | -1.8410203 | 1.6851343 |
| C | 3.3610947 | -2.2987412 | 1.4226666 |
| H | 3.8744006 | -2.9992599 | 2.0946852 |
| C | 4.0180785 | -1.8382003 | 0.2440380 |
| H | 5.0342812 | -2.1959330 | 0.0262979 |
| C | 3.3983839 | -0.9411830 | -0.6437408 |
| H | 3.9329301 | -0.6084100 | -1.5427102 |
| C | 2.0994882 | -0.4725235 | -0.3831001 |
| H | 1.6212462 | 0.2254496 | -1.0811884 |
| C | 1.4331453 | -0.9182253 | 0.7848032 |
| C | -1.4688561 | 0.0152363 | -1.6373830 |
| C | -1.6401408 | -1.3732603 | -1.2853319 |
| H | -1.3439158 | -1.7279529 | -0.2937535 |
| C | -2.1276586 | -2.3265358 | -2.1641812 |
| H | -2.2077614 | -3.3735617 | -1.8427648 |
| C | -2.5297112 | -1.9518830 | -3.4707440 |
| H | -2.9335201 | -2.7006291 | -4.1655021 |
| C | -2.4164365 | -0.6253393 | -3.8562255 |
| H | -2.7397281 | -0.3235405 | -4.8612912 |
| C | -1.8892653 | 0.3839426 | -2.9923887 |
| C | -1.8905200 | 1.6937438 | -3.5546199 |
| H | -2.3540175 | 1.7593284 | -4.5498502 |
| C | -1.3874697 | 2.8841457 | -3.0685650 |
| H | -1.5262681 | 3.7512834 | -3.7306227 |
| C | -0.6595966 | 3.1643382 | -1.8759288 |

| | | | |
|---|---|---|---|
| C | -0.1645286 | 4.5028103 | -1.7905616 |
| H | -0.4011266 | 5.1913392 | -2.6125466 |
| C | 0.6098315 | 4.9444306 | -0.7291675 |
| H | 0.9814319 | 5.9777046 | -0.7037984 |
| C | 0.9255884 | 4.0409659 | 0.3167184 |
| H | 1.5683094 | 4.3622628 | 1.1472070 |
| C | 0.4178358 | 2.7520717 | 0.3000024 |
| H | 0.7095076 | 2.0974733 | 1.1271753 |
| C | -0.4040514 | 2.2387239 | -0.7691172 |
| H | -1.9123875 | -0.1316046 | 0.9667566 |
| H | -0.9279578 | 1.1775500 | 1.5131638 |

**$SMe_2$**

Energy = -477.8743463673

| | | | |
|---|---|---|---|
| S | -0.1314359 | -0.1258515 | -0.8437726 |
| C | 0.7323881 | 1.3696580 | -0.2628578 |
| C | -1.5400209 | -0.1402774 | 0.3121230 |
| H | 0.0992560 | 2.2717169 | -0.3665239 |
| H | 1.0606501 | 1.2675931 | 0.7893649 |
| H | 1.6265859 | 1.4923970 | -0.8999772 |
| H | -2.1639601 | 0.7678647 | 0.2053814 |
| H | -2.1555444 | -1.0217506 | 0.0577541 |
| H | -1.2039716 | -0.2363826 | 1.3624445 |

**$SMe_2$(AuCl)**

Energy = -1073.946269650

| | | | |
|---|---|---|---|
| Au | 1.1778450 | -1.9187523 | -0.3949884 |
| S | -0.1638133 | -0.0876609 | -0.8721822 |
| Cl | 2.4982088 | -3.7262368 | 0.0410519 |
| C | 0.7428931 | 1.3798306 | -0.2564795 |
| C | -1.5498825 | -0.1444866 | 0.3238743 |
| H | 0.1015071 | 2.2701377 | -0.3840615 |
| H | 1.0345571 | 1.2482276 | 0.7990277 |
| H | 1.6459395 | 1.4787491 | -0.8820028 |
| H | -2.1679142 | 0.7614816 | 0.1909484 |
| H | -2.1443503 | -1.0400150 | 0.0764782 |
| H | -1.1749904 | -0.2212950 | 1.3583340 |

Electronic Supplementary Material (ESI) for Dalton Transactions